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Supporting information for article:

Application of the method for visualization of noncovalent interactions in conformational polymorphs of four organic acids

Pavel A. Pirozhkov, Andrei S. Uhanov and Anton V. Savchenkov

SUPPORTING INFORMATION

Application of the method for visualization of noncovalent interactions in conformational polymorphs of four organic acids

Pavel A. Pirozhkov, Andrei S. Uhanov, Anton V. Savchenkov*

Samara National Research University, Samara, Russian Federation

** E-mail: anton.savchenkov@gmail.com*

The Tables S6–S17 include the following characteristics of interatomic interactions:
- k – the number of pyramids representing interatomic contacts;
- d_{min} and d_{max} (Å) – distances for the shortest and the longest contact respectively;
- S (Å^2) – the total surface area of all faces corresponding to the given type of contacts;
- V (Å^3) – the total volume of all pyramids corresponding to the given type of contacts;
- Δ_S (%) – partial contributions of contacts to the total surface area of the corresponding faces.

Table S1. The values of the angle between the planes of aromatic rings θ_{cycle}

Compound	Crystallographically independent molecule	θ_{cycle}, deg.
I	TOKSAO	3,99
	TOKSAO01 mol A	22,12
	TOKSAO01 mol B	27,01
	TOKSAO02 mol D	41,33
	TOKSAO02 mol A	42,46
	TOKSAO03 mol A	54,61
	TOKSAO02 mol C	57,52
	TOKSAO02 mol B	60,59
	TOKSAO03 mol B	76,90
II	BIXGIY05	1,72
	BIXGIY06	20,13
	FISZUF	40,01
	BIXGIY07	111,96
III	KAXXAI10	44,34
	KAXXAI11	52,33
	KAXXAI02 mol B	53,48
	KAXXAI02 mol A	54,32
	KAXXAI03 mol C	58,13
	KAXXAI05	58,67
	KAXXAI07	59,88
	KAXXAI03 mol A	61,48
	KAXXAI03 mol B	63,78
	KAXXAI04	89,04
	KAXXAI06	104,58
	KAXXAI09	107,18

Table S1 (contiuned)

Compound	Crystallographic type of molecule	θ_{cycle}, grad.
IV	MOTNUF01 mol A	55,10
	MOTNUF03 mol H	57,17
	MOTNUF01 mol B	57,42
	MOTNUF01 mol C	57,98
	MOTNUF02 mol B	58,33
	MOTNUF03 mol J	59,16
	MOTNUF03 mol B	59,27
	MOTNUF02 mol A	60,14
	MOTNUF03 mol C	62,88
	MOTNUF03 mol E	64,21
	MOTNUF	65,56
	MOTNUF02 mol C	70,34
	MOTNUF03 mol D	115,73
	MOTNUF03 mol F	116,8
	MOTNUF03 mol I	120,78
	MOTNUF03 mol A	121,40
	MOTNUF03 mol G	122,29

Table S2. The number of faces representing interatomic contacts in **I** with RF>1

Molecule	Contact							
	H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O
TOKSAO	8	19	8	3	0	1	4	2
TOKSAO01 mol A	7	19	9	4	2	1	4	1
TOKSAO01 mol B	7	19	8	4	2	1	3	1
TOKSAO02 mol A	7	18	8	4	1	1	3	1
TOKSAO02 mol B	7	20	9	4	2	1	3	1
TOKSAO02 mol C	7	21	11	4	2	1	3	3
TOKSAO02 mol D	7	21	8	4	1	1	3	2
TOKSAO03 mol A	7	19	8	4	3	1	3	1
TOKSAO03 mol B	8	20	9	5	2	1	3	1

Table S3. The number of faces representing interatomic contacts in **II** with RF>1

Molecule	Contact											
	H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	H/Cl	C/Cl
BIXGIY07	10	25	9	6	5	1	3	1	0	0	3	1
FISZUF	10	25	7	4	2	0	3	2	0	1	3	1
BIXGIY06	9	22	8	4	2	1	5	1	0	0	2	0
BIXGIY05	9	21	8	3	0	1	5	1	0	0	2	0

Table S4. The number of faces representing interatomic contacts in **III** with RF>1

Molecule	Contact									
	H/H	H/C	C/C	H/N	C/N	H/O	C/O	O/O	H/Cl	C/Cl
KAXXAI09	13	31	9	3	0	3	1	0	3	1
KAXXAI10	11	29	10	3	1	5	1	0	3	1
KAXXAI02 mol A	11	29	11	3	0	3	1	0	3	0
KAXXAI02 mol B	12	32	7	3	2	5	2	0	2	0
KAXXAI03 mol A	12	32	9	3	0	4	1	0	3	1
KAXXAI03 mol B	12	31	10	3	1	3	1	0	3	1
KAXXAI03 mol C	11	30	9	3	0	3	1	0	3	0
KAXXAI04	13	32,5	12	3,5	1,5	3	1	1	3	1
KAXXAI07	12	31	9	3	1	3	1	0	3	0
KAXXAI05	12	30	8	3	1	4	1	0	3	0
KAXXAI06	12	34	17	4	1	3	1	0	3	0
KAXXAI11	11	29	7	3	0	4	1	0	3	1

Table S5. The number of faces representing interatomic contacts in **IV** with RF>1

Molecule	Contact									
	H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O
MOTNUF	11	24	18	8	3	1	4	8	1	0
MOTNUF01 mol A	12	26	19	8	4	1	5	8	1	0
MOTNUF01 mol B	10	27	20	9	4	1	4	9	1	0
MOTNUF01 mol C	12	27	18	9	3	1	5	9	1	0
MOTNUF02 mol A	13	27	21	8	4	1	5	9	1	0
MOTNUF02 mol B	12	28	16	9	3	1	5	8	1	0
MOTNUF02 mol C	11	27	16	9	3	1	4	7	1	0
MOTNUF03 mol A	12	24	16	9	4	1	5	7	1	0
MOTNUF03 mol B	12	26	17	9	3	1	5	8	1	0
MOTNUF03 mol C	13	26	17	8	4	1	5	9	1	0
MOTNUF03 mol D	13	27	14	8	4	1	5	9	1	0
MOTNUF03 mol E	13	26	19	8	3	1	5	9	1	0
MOTNUF03 mol F	13	27	18	8	3	1	5	9	1	0
MOTNUF03 mol G	11	27	18	8	4	1	4	7	1	0
MOTNUF03 mol H	11	26	17	8	4	1	4	7	1	0
MOTNUF03 mol I	10	27	16	9	3	1	4	9	1	0
MOTNUF03 mol J	10	27	20	9	3	1	4	9	1	1

Table S6. Characteristics of chemical bonds in 2-(phenylamino)nicotinic acid (**I**) polymorphs (VD polyhedra faces with RF = 1)

		H/C	C/C	H/N	C/N	H/O	C/O	∑
TOKSAO	*k*	16	22	2	8	2	4	54
	d_{min}	0,95	1,38	0,88	1,33	0,84	1,24	0,84
	d_{max}	0,95	1,47	0,88	1,41	0,84	1,32	1,47
	S	111,52	139,96	11,34	51,89	13,43	24,46	352,59
	V	17,66	32,68	1,66	11,79	1,88	5,21	70,89
	Δ_S	31,63	39,69	3,22	14,72	3,81	6,94	100,00
TOKSAO01	*k*	16	22	2	8	2	4	54
	d_{min}	0,95	1,38	0,88	1,33	0,84	1,24	0,84
	d_{max}	0,95	1,47	0,88	1,42	0,84	1,32	1,47
	S	112,88	147,92	11,98	51,49	13,86	24,12	362,24
	V	17,87	34,50	1,76	11,70	1,94	5,13	72,90
	Δ_S	31,16	40,83	3,31	14,21	3,83	6,66	100,00
Mol A	*k*	16	22	2	8	2	4	54
	d_{min}	0,95	1,38	0,88	1,33	0,84	1,24	0,84
	d_{max}	0,95	1,47	0,88	1,42	0,84	1,32	1,47
	S	112,18	150,12	12,88	51,79	13,35	24,20	364,52
	V	17,76	35,00	1,89	11,77	1,87	5,15	73,43
	Δ_S	30,78	41,18	3,53	14,21	3,66	6,64	100,00
Mol B	*k*	16	22	2	8	2	4	54
	d_{min}	0,95	1,38	0,88	1,33	0,84	1,24	0,84
	d_{max}	0,95	1,47	0,88	1,41	0,84	1,32	1,47
	S	113,57	145,72	11,07	51,19	14,37	24,05	359,98
	V	17,98	34,00	1,63	11,63	2,01	5,12	72,36
	Δ_S	31,55	40,48	3,08	14,22	3,99	6,68	100,00
TOKSAO02	*k*	16	22	2	8	2	4	54
	d_{min}	0,95	1,37	0,88	1,34	0,84	1,22	0,84
	d_{max}	0,95	1,49	0,88	1,42	0,84	1,32	1,49
	S	108,28	147,06	12,54	50,51	14,51	24,36	357,25
	V	17,14	34,18	1,84	11,45	2,03	5,13	71,78
	Δ_S	30,31	41,16	3,51	14,14	4,06	6,82	100,00
Mol A	*k*	16	22	2	8	2	4	54
	d_{min}	0,95	1,38	0,88	1,34	0,84	1,23	0,84
	d_{max}	0,95	1,48	0,88	1,40	0,84	1,31	1,48
	S	107,30	145,83	12,29	51,23	14,83	25,17	356,65
	V	16,98	33,92	1,80	11,61	2,08	5,31	71,70
	Δ_S	30,08	40,89	3,45	14,36	4,16	7,06	100,00
Mol B	*k*	16	22	2	8	2	4	54
	d_{min}	0,95	1,38	0,88	1,34	0,84	1,22	0,84
	d_{max}	0,95	1,48	0,88	1,42	0,84	1,32	1,48
	S	111,85	150,68	13,03	50,56	14,03	24,24	364,39
	V	17,71	34,99	1,91	11,46	1,96	5,11	73,15
	Δ_S	30,70	41,35	3,58	13,88	3,85	6,65	100,00

Table S6 (continued)

		H/C	C/C	H/N	C/N	H/O	C/O	∑
Mol C	*k*	16	22	2	8	2	4	54
	d_{min}	0,95	1,37	0,88	1,34	0,84	1,22	0,84
	d_{max}	0,95	1,48	0,88	1,42	0,84	1,32	1,48
	S	108,05	146,47	12,61	48,75	14,35	23,26	353,49
	V	17,11	34,04	1,85	11,05	2,01	4,90	70,96
	Δ_S	30,57	41,44	3,57	13,79	4,06	6,58	100,00
Mol D	*k*	16	22	2	8	2	4	54
	d_{min}	0,95	1,37	0,88	1,34	0,84	1,23	0,84
	d_{max}	0,95	1,49	0,88	1,41	0,84	1,31	1,49
	S	105,92	145,24	12,23	51,51	14,81	24,76	354,48
	V	16,77	33,78	1,79	11,67	2,07	5,21	71,30
	Δ_S	29,88	40,97	3,45	14,53	4,18	6,99	100,00
TOKSAO03	*k*	16	22	2	8	2	4	54
	d_{min}	0,95	1,37	0,88	1,33	0,84	1,22	0,84
	d_{max}	0,95	1,49	0,88	1,42	0,84	1,32	1,49
	S	109,70	150,99	12,96	51,85	15,06	24,14	364,69
	V	17,37	35,15	1,90	11,76	2,11	5,08	73,36
	Δ_S	30,08	41,40	3,55	14,22	4,13	6,62	100,00
Mol A	*k*	16	22	2	8	2	4	54
	d_{min}	0,95	1,37	0,88	1,33	0,84	1,22	0,84
	d_{max}	0,95	1,49	0,88	1,42	0,84	1,32	1,49
	S	110,29	155,33	12,58	53,18	14,53	22,77	368,68
	V	17,46	36,15	1,85	12,08	2,03	4,80	74,36
	Δ_S	29,92	42,13	3,41	14,42	3,94	6,18	100,00
Mol B	*k*	16	22	2	8	2	4	54
	d_{min}	0,95	1,37	0,88	1,34	0,84	1,23	0,84
	d_{max}	0,95	1,49	0,88	1,42	0,84	1,31	1,49
	S	109,10	146,64	13,33	50,52	15,60	25,50	360,69
	V	17,28	34,15	1,96	11,44	2,18	5,37	72,37
	Δ_S	30,25	40,66	3,70	14,01	4,32	7,07	100,00

Table S7. Characteristics of chemical bonds in 2-(phenylamino)nicotinic acid (**I**) polymorphs (VD polyhedra faces with RF > 1)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
TOKSAO	*k*	16	38	16	6		2	8	4			90
	d_{min}	2,20	1,79	2,30	1,96		2,33	1,96	2,35			1,79
	d_{max}	3,61	2,63	2,76	2,72		2,33	3,59	2,39			3,61
	S	43,65	13,50	1,26	16,96		1,09	26,66	0,30			103,41
	V	16,94	4,59	0,51	6,33		0,42	9,58	0,12			38,49
	Δ_S	42,21	13,05	1,22	16,40		1,05	25,78	0,29			100,00
TOKSAO01	*k*	14	38	17	8	4	2	7	2			92
	d_{min}	2,28	1,79	2,31	1,96	2,92	2,32	1,97	2,34			1,79
	d_{max}	2,35	2,94	2,76	2,70	2,94	2,33	3,71	2,34			3,71
	S	44,08	14,53	1,34	12,86	0,89	1,07	23,81	0,32			98,89
	V	17,08	5,03	0,53	5,01	0,43	0,41	8,50	0,13			37,13
	Δ_S	44,58	14,69	1,36	13,00	0,89	1,08	24,08	0,32			100,00
Mol A	*k*	14	38	18	8	4	2	8	2			94
	d_{min}	2,28	1,79	2,31	1,96	2,92	2,32	1,97	2,34			1,79
	d_{max}	2,35	2,94	2,76	2,70	2,93	2,32	3,71	2,34			3,71
	S	42,73	14,64	1,29	12,79	0,78	0,95	25,76	0,29			99,22
	V	16,55	5,03	0,51	5,00	0,38	0,37	9,17	0,11			37,11
	Δ_S	43,07	14,75	1,30	12,89	0,79	0,96	25,96	0,29			100,00
Mol B	*k*	14	38	16	8	4	2	6	2			90
	d_{min}	2,28	1,79	2,31	1,96	2,92	2,33	1,99	2,34			1,79
	d_{max}	2,35	2,89	2,76	2,70	2,94	2,33	2,37	2,34			2,94
	S	45,44	14,42	1,40	12,93	0,99	1,18	21,88	0,35			98,58
	V	17,62	5,04	0,55	5,03	0,48	0,46	7,84	0,14			37,15
	Δ_S	46,09	14,63	1,42	13,12	1,00	1,20	22,19	0,35			100,00
TOKSAO02	*k*	14	40	18	8	3	2	6	3,5			94,5
	d_{min}	2,31	1,77	2,31	1,97	2,85	2,32	1,90	2,33			1,77
	d_{max}	2,62	3,02	2,77	2,88	3,13	2,34	2,37	2,67			3,13
	S	40,94	15,43	1,21	9,46	0,89	1,09	25,55	0,63			95,21
	V	16,08	5,45	0,48	4,07	0,43	0,42	9,22	0,24			36,39

	Δ_S	43,00	16,21	1,27	9,94	0,94	1,14	26,84	0,66	100,00
Mol A	k	14	36	16	8	2	2	6	2	86
	d_{min}	2,31	1,78	2,31	1,97	2,95	2,34	1,90	2,33	1,78
	d_{max}	2,36	2,94	2,75	2,68	2,95	2,34	2,37	2,33	2,95
	S	41,26	16,02	1,25	8,54	0,58	1,28	26,21	0,65	95,78
	V	16,07	5,59	0,50	3,60	0,29	0,50	9,35	0,25	36,15
	Δ_S	43,07	16,72	1,31	8,91	0,61	1,34	27,36	0,67	100,00
Mol B	k	14	40	18	8	4	2	6	2	94
	d_{min}	2,31	1,78	2,31	1,97	2,86	2,32	1,99	2,33	1,78
	d_{max}	2,57	2,94	2,76	2,88	3,13	2,32	2,35	2,33	3,13
	S	41,59	15,79	1,06	10,85	0,85	1,50	25,09	0,54	97,26
	V	16,39	5,61	0,42	4,72	0,40	0,58	9,14	0,21	37,47
	Δ_S	42,76	16,23	1,09	11,16	0,87	1,54	25,79	0,56	100,00

Table S7 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	Σ
Mol C	*k*	14	42	22	8	4	2	6	6			104
	d_{min}	2,31	1,78	2,31	1,97	2,85	2,32	1,98	2,33			1,78
	d_{max}	2,62	3,02	2,77	2,86	3,10	2,32	2,35	2,67			3,10
	S	38,74	14,65	1,25	9,30	1,31	0,66	24,69	0,83			91,43
	V	15,31	5,25	0,50	4,06	0,62	0,26	8,97	0,32			35,28
	Δ_S	42,37	16,03	1,36	10,17	1,43	0,73	27,01	0,91			100,00
Mol D	*k*	14	42	16	8	2	2	6	4			94
	d_{min}	2,31	1,77	2,31	1,97	2,92	2,33	1,93	2,33			1,77
	d_{max}	2,45	2,99	2,75	2,69	2,92	2,33	2,35	2,39			2,99
	S	42,19	15,28	1,27	9,17	0,85	0,90	26,22	0,50			96,37
	V	16,53	5,35	0,50	3,90	0,41	0,35	9,42	0,19			36,66
	Δ_S	43,78	15,85	1,32	9,51	0,88	0,93	27,21	0,52			100,00
TOKSAO03	*k*	15	39	17	9	5	2	6	2			95
	d_{min}	2,32	1,77	2,30	1,96	2,41	2,31	1,99	2,33			1,77
	d_{max}	3,17	3,13	2,76	3,90	3,28	2,33	2,36	2,33			3,90
	S	37,03	17,37	1,36	10,82	1,05	1,36	26,34	0,71			96,05
	V	14,63	6,25	0,54	4,68	0,50	0,53	9,57	0,28			36,97
	Δ_S	38,56	18,09	1,42	11,27	1,09	1,42	27,43	0,74			100,00
Mol A	*k*	14	38	16	8	6	2	6	2			92
	d_{min}	2,32	1,78	2,31	1,96	2,41	2,33	1,99	2,33			1,78
	d_{max}	2,50	2,89	2,76	2,77	3,08	2,33	2,36	2,33			3,08
	S	37,30	17,49	1,27	10,53	0,71	1,65	26,90	0,73			96,57
	V	14,72	6,43	0,50	4,52	0,34	0,64	9,75	0,29			37,19
	Δ_S	38,62	18,11	1,31	10,90	0,74	1,71	27,86	0,76			100,00
Mol B	*k*	16	40	18	10	4	2	6	2			98
	d_{min}	2,32	1,77	2,30	1,97	2,80	2,31	1,99	2,33			1,77
	d_{max}	3,17	3,13	2,76	3,90	3,28	2,31	2,36	2,33			3,90
	S	36,77	17,26	1,46	11,12	1,38	1,07	25,78	0,68			95,53
	V	14,53	6,08	0,58	4,85	0,65	0,41	9,40	0,27			36,75
	Δ_S	38,49	18,06	1,53	11,64	1,45	1,12	26,99	0,72			100,00

Table S8. Characteristics of chemical bonds in 2-(phenylamino)nicotinic acid (**I**) polymorphs (VD polyhedra faces with RF = 0)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
TOKSAO	*k*	71	112	15	20	2		18	18	2	2	260
	d_{min}	2,52	2,79	3,30	2,74	4,16		1,80	3,33	3,69	3,77	1,80
	d_{max}	4,47	4,02	3,77	4,09	4,16		4,04	3,97	3,69	3,77	4,47
	S	98,17	101,41	2,32	23,42	0,01		40,41	10,02	1,20	0,27	277,23
	V	49,48	54,40	1,30	12,07	0,01		17,99	5,64	0,74	0,17	141,80
	Δ_S	35,41	36,58	0,84	8,45	0,00		14,58	3,61	0,43	0,10	100,00
TOKSAO01	*k*	72	107	13	9	15	1	16	23	6	3	265
	d_{min}	2,32	2,79	3,34	2,53	3,20	3,68	1,82	3,12	3,33	3,37	1,82
	d_{max}	4,93	4,52	3,82	4,15	4,25	3,68	3,96	3,94	3,59	3,58	4,93
	S	118,37	84,41	2,28	13,23	10,06	0,11	33,80	14,37	3,25	0,40	280,27
	V	58,92	46,93	1,36	6,41	5,72	0,07	14,26	8,15	1,87	0,24	143,92
	Δ_S	42,24	30,12	0,81	4,72	3,59	0,04	12,06	5,13	1,16	0,14	100,00
Mol A	*k*	70	109	13	9	15	1	15	23	6	3	264
	d_{min}	2,32	2,79	3,34	2,56	3,20	3,68	1,82	3,12	3,33	3,37	1,82
	d_{max}	4,38	4,53	3,82	4,15	4,25	3,68	3,96	3,94	3,59	3,58	4,53
	S	116,69	84,01	2,27	12,94	10,06	0,11	33,47	14,37	3,25	0,40	277,57
	V	57,41	46,72	1,36	6,29	5,72	0,07	14,11	8,15	1,87	0,24	141,93
	Δ_S	42,04	30,27	0,82	4,66	3,62	0,04	12,06	5,18	1,17	0,15	100,00
Mol B	*k*	74	105	13	9	15	1	17	23	6	3	266
	d_{min}	2,33	2,79	3,34	2,53	3,20	3,68	1,83	3,12	3,33	3,37	1,83
	d_{max}	4,93	4,53	3,82	4,15	4,25	3,68	3,96	3,94	3,59	3,58	4,93
	S	120,06	84,80	2,27	13,53	10,06	0,11	34,12	14,37	3,25	0,40	282,97
	V	60,44	47,14	1,36	6,52	5,72	0,07	14,41	8,15	1,87	0,24	145,91
	Δ_S	42,43	29,97	0,80	4,78	3,55	0,04	12,06	5,08	1,15	0,14	100,00
TOKSAO02	*k*	76	85	32,5	17,5	7,5	1,333	17,5	21	7,5	1	266,83
	d_{min}	2,30	2,72	3,32	1,81	3,38	3,79	2,43	2,91	3,12	3,49	1,81
	d_{max}	5,00	4,63	4,01	4,15	3,99	3,80	4,02	4,22	3,81	3,49	5,00
	S	132,47	63,61	14,41	18,53	2,91	0,24	31,78	13,48	5,40	0,21	283,05
	V	68,09	34,54	8,44	7,63	1,72	0,15	14,74	7,61	3,06	0,12	146,09
	Δ_S	46,80	22,47	5,09	6,55	1,03	0,09	11,23	4,76	1,91	0,08	100,00
Mol A	*k*	76	87	24	18	5		18	18	10		256
	d_{min}	2,38	2,72	3,33	1,85	3,41		2,43	2,96	3,31		1,85
	d_{max}	4,76	4,63	3,91	4,15	3,81		4,02	3,74	3,77		4,76
	S	134,41	65,28	10,23	18,18	2,41		29,30	13,80	7,04		280,64
	V	68,01	35,37	5,96	7,60	1,41		13,40	7,65	4,04		143,42
	Δ_S	47,89	23,26	3,64	6,48	0,86		10,44	4,92	2,51		100,00
Mol B	*k*	76	90	41	20	7	1	17	20	9		281
	d_{min}	2,43	2,74	3,33	1,81	3,41	3,79	2,45	2,91	3,31		1,81
	d_{max}	4,57	4,28	4,01	4,15	3,99	3,79	4,02	4,07	3,77		4,57
	S	125,82	67,38	16,89	19,06	2,67	0,43	30,57	14,90	7,01		284,73
	V	66,48	37,31	9,94	7,69	1,57	0,27	14,19	8,30	4,02		149,78
	Δ_S	44,19	23,66	5,93	6,69	0,94	0,15	10,74	5,23	2,46		100,00

Table S8 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
Mol C	*k*	76	80	40	17	10	2	18	22	6	1	272
	d_{min}	2,30	2,72	3,32	1,85	3,38	3,79	2,43	2,96	3,12	3,49	1,85
	d_{max}	5,00	4,23	3,84	4,14	3,99	3,80	3,62	4,22	3,81	3,49	5,00
	S	130,36	61,09	17,97	17,92	3,42	0,49	36,44	12,06	3,78	0,43	283,97
	V	66,53	33,07	10,48	7,41	2,03	0,31	17,04	6,92	2,09	0,25	146,14
	Δ_S	45,91	21,51	6,33	6,31	1,20	0,17	12,83	4,25	1,33	0,15	100,00
Mol D	*k*	76	80	40	17	10	2	18	22	6	1	272
	d_{min}	2,30	2,72	3,32	1,85	3,38	3,79	2,43	2,96	3,12	3,49	1,85
	d_{max}	5,00	4,23	3,84	4,14	3,99	3,80	3,62	4,22	3,81	3,49	5,00
	S	130,36	61,09	17,97	17,92	3,42	0,49	36,44	12,06	3,78	0,43	283,97
	V	66,53	33,07	10,48	7,41	2,03	0,31	17,04	6,92	2,09	0,25	146,14
	Δ_S	45,91	21,51	6,33	6,31	1,20	0,17	12,83	4,25	1,33	0,15	100,00
TOKSAO03	*k*	76	96	13	14	12		18	31	5		265
	d_{min}	2,41	2,72	3,29	1,83	3,61		2,43	3,00	3,34		1,83
	d_{max}	4,50	4,47	4,30	4,29	4,34		3,85	4,36	3,72		4,50
	S	124,95	79,20	5,78	17,90	2,19		31,46	15,97	6,47		283,92
	V	62,41	42,90	3,47	7,02	1,41		14,89	9,44	3,76		145,30
	Δ_S	44,01	27,89	2,04	6,30	0,77		11,08	5,63	2,28		100,00
Mol A	*k*	73	89	17	18	17		20	29	5		268
	d_{min}	2,41	2,72	3,29	1,83	3,72		2,43	3,00	3,47		1,83
	d_{max}	4,50	4,47	4,12	4,29	4,34		3,85	4,36	3,72		4,50
	S	125,68	74,02	5,88	20,74	3,65		33,15	15,04	5,17		283,33
	V	62,73	40,45	3,68	8,70	2,35		15,86	8,93	3,07		145,77
	Δ_S	44,36	26,13	2,07	7,32	1,29		11,70	5,31	1,83		100,00
Mol B	*k*	79	103	9	10	7		16	33	5		262
	d_{min}	2,41	2,72	3,29	1,83	3,61		2,43	3,00	3,34		1,83
	d_{max}	4,50	4,47	4,30	3,87	4,03		3,85	4,36	3,72		4,50
	S	124,22	84,37	5,69	15,06	0,73		29,77	16,91	7,76		284,51
	V	62,09	45,34	3,26	5,34	0,46		13,91	9,95	4,46		144,82
	Δ_S	43,66	29,65	2,00	5,29	0,26		10,46	5,94	2,73		100,00

Table S9. Characteristics of chemical bonds in 2-(3-chloro-2-methylphenylamino)nicotinic acid (**II**) polymorphs (VD polyhedra faces with RF = 1)

		H/C	C/C	H/N	C/N	H/O	C/O	C/Cl	∑
BIXGIY07	*k*	18	24	2	8	2	4	2	60
	d_{min}	0,95	1,38	0,88	1,35	0,84	1,22	1,75	0,84
	d_{max}	0,98	1,50	0,88	1,43	0,84	1,32	1,75	1,75
	S	106,44	155,73	11,09	48,73	14,98	23,37	13,88	374,22
	V	16,95	36,45	1,63	11,10	2,10	4,93	4,04	77,19
	Δ_S	28,44	41,62	2,96	13,02	4,00	6,24	3,71	100,00
FISZUF	*k*	18	24	4	8		4	2	60
	d_{min}	0,95	1,36	0,88	1,34		1,26	1,75	0,88
	d_{max}	0,98	1,52	0,88	1,42		1,26	1,75	1,75
	S	104,21	160,85	25,00	49,69		29,78	13,92	383,46
	V	16,60	37,70	3,67	11,32		6,24	4,07	79,59
	Δ_S	27,18	41,95	6,52	12,96		7,77	3,63	100,00
BIXGIY06	*k*	18	24	2	8	2	4	2	60
	d_{min}	0,95	1,38	0,86	1,33	0,85	1,24	1,75	0,85
	d_{max}	0,98	1,51	0,86	1,41	0,85	1,32	1,75	1,75
	S	104,26	159,79	12,56	52,72	16,09	25,05	13,30	383,78
	V	16,60	37,44	1,79	11,98	2,29	5,33	3,88	79,30
	Δ_S	27,17	41,64	3,27	13,74	4,19	6,53	3,47	100,00
BIXGIY05	*k*	18	24	2	8	2	4	2	60
	d_{min}	0,95	1,38	0,88	1,34	0,87	1,24	1,75	0,87
	d_{max}	0,98	1,51	0,88	1,41	0,87	1,32	1,75	1,75
	S	104,12	154,45	13,22	50,30	16,31	24,60	14,05	377,04
	V	16,58	36,16	1,94	11,43	2,36	5,23	4,09	77,79
	Δ_S	27,61	40,96	3,51	13,34	4,33	6,53	3,73	100,00

Table S10. Characteristics of chemical bonds in 2-(3-chloro-2-methylphenylamino)nicotinic acid (**II**) polymorphs (VD polyhedra faces with RF > 1)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	H/Cl	C/Cl	N/Cl	O/Cl	Cl/Cl	∑
BIXGIY07	*k*	20	50	18	12	10	2	6	2			6	2				128
	d_{min}	1,60	1,79	2,32	1,98	2,45	2,32	1,94	2,35			2,687	3,051				1,60
	d_{max}	3,86	4,22	2,74	4,01	3,23	2,32	2,41	2,35			3,242	3,051				4,22
	S	48,04	32,82	1,73	15,23	1,57	1,06	27,47	0,493			14,237	0,017				142,66
	V	17,43	12,22	0,70	6,66	0,75	0,41	9,95	0,193			6,546	0,009				54,85
	Δ_S	33,67	23,01	1,21	10,67	1,10	0,75	19,25	0,35			9,98	0,01				100,00
FISZUF	*k*	20	50	14	8	4		6	4		2	6	2				116
	d_{min}	1,60	1,89	2,37	2,39	2,38		1,82	2,362		2,238	2,773	3,044				1,60
	d_{max}	2,36	2,93	2,75	2,68	2,72		2,67	2,384		2,238	2,938	3,044				3,04
	S	57,10	32,49	1,43	6,00	0,47		21,94	0,035		0,809	15,367	0,048				135,68
	V	19,45	12,03	0,57	2,54	0,20		8,00	0,014		0,302	7,336	0,025				50,47
	Δ_S	42,08	23,94	1,05	4,42	0,34		16,17	0,03		0,60	11,33	0,04				100,00
BIXGIY06	*k*	18	44	16	8	4	2	10	2			4					108
	d_{min}	1,60	1,79	2,30	1,97	2,88	2,33	1,97	2,344			2,551					1,60
	d_{max}	2,35	2,85	2,76	2,67	2,93	2,33	3,11	2,344			2,759					3,11
	S	45,09	27,40	1,90	13,63	0,69	1,06	27,49	0,352			11,772					129,38
	V	15,26	9,70	0,75	5,20	0,34	0,41	10,62	0,138			5,15					47,56
	Δ_S	34,85	21,18	1,47	10,54	0,53	0,82	21,25	0,27			9,10					100,00
BIXGIY05	*k*	18	42	16	6		2	10	2			4					100
	d_{min}	1,60	1,78	2,30	1,97		2,34	1,93	2,351			2,527					1,60
	d_{max}	2,34	2,81	2,76	2,69		2,34	2,98	2,351			2,757					2,98
	S	47,75	28,18	1,70	13,08		0,80	28,53	0,264			14,178					134,49
	V	15,94	9,92	0,67	4,92		0,31	10,88	0,103			6,16					48,91
	Δ_S	35,50	20,95	1,27	9,73		0,60	21,21	0,20			10,54					100,00

Table S11. Characteristics of chemical bonds in 2-(3-chloro-2-methylphenylamino)nicotinic acid (**II**) polymorphs (VD polyhedra faces with RF = 0)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	H/Cl	C/Cl	N/Cl	O/Cl	Cl/Cl	∑
BIXGIY07	*k*	64	90	16	12			18	18		2	24	6	2	6		258
	d_{min}	2,49	2,80	3,55	1,86			2,35	3,076		4,625	3,039	3,338	4,046	3,433		1,86
	d_{max}	4,38	4,57	4,03	3,95			4,61	3,665		4,625	4,66	4,197	4,046	3,483		4,66
	S	118,55	70,90	9,68	21,11			32,89	11,455		0,866	39,628	5,819	0,692	11,353		322,94
	V	60,07	38,26	5,93	8,51			15,22	6,492		0,668	22,921	3,35	0,466	6,555		168,44
	Δ_S	36,71	21,95	3,00	6,54			10,18	3,55		0,27	12,27	1,80	0,21	3,52		100,00
FISZUF	*k*	64	76	62	10	10		24	22	6	2	14	6			2	298
	d_{min}	2,58	2,88	3,35	3,55	3,36		1,91	3,039	3,326	3,935	2,923	3,622			3,935	1,91
	d_{max}	4,51	4,12	4,15	3,98	3,64		3,93	4,116	3,557	3,935	3,681	4,134			3,935	4,51
	S	108,33	39,13	23,44	4,22	5,40		53,46	10,935	3,729	0,154	43,03	5,324			0,888	298,03
	V	54,47	22,42	14,02	2,54	3,09		22,08	6,172	2,123	0,101	22,532	3,238			0,583	153,37
	Δ_S	36,35	13,13	7,86	1,42	1,81		17,94	3,67	1,25	0,05	14,44	1,79			0,30	100,00
BIXGIY06	*k*	61	68	66	6	24	4	16	10	2	7	20	4		4	2	294
	d_{min}	2,41	2,84	3,42	2,78	3,39	3,79	1,80	3,35	3,65	3,445	2,943	3,657		3,277	3,785	1,80
	d_{max}	3,86	4,29	4,20	3,64	3,95	3,79	3,99	3,811	3,65	3,785	3,955	3,719		4,123	3,785	4,29
	S	118,44	37,77	26,30	11,81	12,44	0,68	30,36	6,357	0,241	2,137	36,664	3,726		8,36	2,962	298,23
	V	55,26	21,70	15,78	5,79	7,48	0,43	13,27	3,638	0,147	1,288	19,859	2,278		4,825	1,868	153,61
	Δ_S	39,71	12,66	8,82	3,96	4,17	0,23	10,18	2,13	0,08	0,72	12,29	1,25		2,80	0,99	100,00
BIXGIY05	*k*	67	64	48	14	16	4	18	24	6		26	4		2	1	294
	d_{min}	2,32	2,77	3,34	2,74	3,54	3,56	1,82	3,422	3,467		2,901	3,814		3,454	3,897	1,82
	d_{max}	4,22	4,00	3,98	3,84	3,96	3,73	3,70	3,865	3,542		4,288	4,011		3,454	3,897	4,29
	S	111,50	44,13	26,56	15,62	3,98	1,71	29,66	9,281	3,596		43,702	2,018		5,21	1,233	298,21
	V	53,58	23,75	15,61	8,03	2,39	1,02	13,48	5,608	2,101		24,157	1,305		2,999	0,8	154,82
	Δ_S	37,39	14,80	8,91	5,24	1,34	0,57	9,95	3,11	1,21		14,65	0,68		1,75	0,41	100,00

Table S12. Characteristics of chemical bonds in *N*-(3-chloro-2-methylphenyl)anthranilic acid (**III**) polymorphs (VD polyhedra faces with RF = 1)

		H/C	C/C	H/N	C/N	H/O	C/O	C/Cl	∑
KAXXAI09	*k*	20	28	2	4	2	4	2	62
	d_{min}	1,052	1,378	1,021	1,365	1,021	1,239	1,738	1,02
	d_{max}	1,094	1,497	1,021	1,418	1,021	1,316	1,738	1,74
	S	114,905	188,608	12,795	21,334	14,612	26,307	13,642	392,20
	V	20,756	44,188	2,178	4,944	2,486	5,594	3,952	84,10
	Δ_S	29,297	48,090	3,262	5,440	3,726	6,708	3,478	100,00
KAXXAI10	*k*	20	28	2	4	2	4	2	62
	d_{min}	1,046	1,378	1,019	1,369	0,998	1,236	1,737	1,00
	d_{max}	1,087	1,497	1,019	1,400	0,998	1,314	1,737	1,74
	S	118,865	194,221	12,400	24,660	17,109	27,329	14,382	408,97
	V	21,324	45,456	2,107	5,686	2,846	5,795	4,164	87,38
	Δ_S	29,065	47,491	3,032	6,030	4,183	6,682	3,517	100,00
KAXXAI02	*k*	20	28	2	4	2	4	2	62
	d_{min}	0,929	1,375	0,860	1,368	0,834	1,236	1,736	0,83
	d_{max}	0,961	1,501	0,861	1,407	0,845	1,317	1,740	1,74
	S	114,525	177,132	12,228	22,509	14,340	25,226	14,522	380,48
	V	17,844	41,445	1,753	5,200	2,007	5,363	4,206	77,82
	Δ_S	30,100	46,555	3,214	5,916	3,769	6,630	3,817	100,00
Mol A	*k*	20	28	2	4	2	4	2	62
	d_{min}	0,929	1,375	0,860	1,370	0,834	1,239	1,736	0,83
	d_{max}	0,961	1,501	0,860	1,407	0,834	1,316	1,736	1,74
	S	112,928	178,727	12,338	22,256	14,166	24,987	14,420	379,82
	V	17,598	41,807	1,768	5,147	1,969	5,317	4,171	77,78
	Δ_S	29,732	47,055	3,248	5,860	3,730	6,579	3,797	100,00
Mol B	*k*	20	28	2	4	2	4	2	62
	d_{min}	0,929	1,377	0,861	1,368	0,845	1,236	1,740	0,85
	d_{max}	0,960	1,501	0,861	1,405	0,845	1,317	1,740	1,74
	S	116,122	175,538	12,119	22,763	14,514	25,465	14,625	381,15
	V	18,090	41,082	1,738	5,252	2,044	5,410	4,241	77,86
	Δ_S	30,467	46,055	3,180	5,972	3,808	6,681	3,837	100,00
KAXXAI03	*k*	20	28	2	4	2	4	2	62
	d_{min}	0,949	1,371	0,865	1,365	0,836	1,234	1,745	0,84
	d_{max}	0,981	1,505	0,877	1,424	0,863	1,317	1,747	1,75
	S	116,572	176,958	11,697	22,045	13,641	24,967	14,719	380,60
	V	18,549	41,346	1,699	5,114	1,931	5,298	4,282	78,22
	Δ_S	30,628	46,494	3,073	5,792	3,584	6,560	3,867	100,00
Mol A	*k*	20	28	2	4	2	4	2	62
	d_{min}	0,949	1,375	0,873	1,372	0,863	1,236	1,745	0,86
	d_{max}	0,981	1,505	0,873	1,420	0,863	1,313	1,745	1,75
	S	115,379	176,890	11,139	21,859	13,756	25,268	14,691	378,98
	V	18,357	41,343	1,620	5,078	1,979	5,362	4,273	78,01
	Δ_S	30,444	46,675	2,939	5,768	3,630	6,667	3,876	100,00

Table S12 (continued)

		H/C	C/C	H/N	C/N	H/O	C/O	C/Cl	∑
Mol B	*k*	20	28	2	4	2	4	2	62
	d_{min}	0,949	1,374	0,877	1,365	0,850	1,234	1,745	0,85
	d_{max}	0,980	1,505	0,877	1,424	0,850	1,317	1,745	1,75
	S	118,934	179,936	11,814	21,735	12,642	25,002	15,180	385,24
	V	18,926	42,021	1,728	5,042	1,791	5,311	4,414	79,23
	Δ_S	30,872	46,707	3,067	5,642	3,282	6,490	3,940	100,00
Mol C	*k*	20	28	2	4	2	4	2	62
	d_{min}	0,949	1,371	0,865	1,369	0,836	1,234	1,747	0,84
	d_{max}	0,980	1,493	0,865	1,415	0,836	1,316	1,747	1,75
	S	115,404	174,048	12,136	22,542	14,526	24,631	14,288	377,58
	V	18,363	40,673	1,750	5,220	2,023	5,221	4,160	77,41
	Δ_S	30,565	46,096	3,214	5,970	3,847	6,523	3,784	100,00
KAXXAI04	*k*	20	28	2	4	2	4	2	62
	d_{min}	0,930	1,369	0,874	1,367	0,881	1,238	1,739	0,87
	d_{max}	0,960	1,491	0,914	1,720	0,887	1,320	1,742	1,74
	S	115,728	178,403	10,836	18,572	13,946	23,744	13,305	374,53
	V	18,031	41,562	1,614	4,703	2,055	5,049	3,859	76,87
	Δ_S	30,899	47,634	2,893	4,959	3,723	6,340	3,552	100,00
KAXXAI07	*k*	20	28	2	4	2	4	2	62
	d_{min}	0,930	1,369	0,860	1,369	0,820	1,240	1,731	0,82
	d_{max}	0,960	1,471	0,860	1,425	0,820	1,316	1,731	1,73
	S	116,097	176,305	12,439	22,294	13,554	25,563	15,233	381,49
	V	18,085	41,192	1,783	5,178	1,853	5,437	4,395	77,92
	Δ_S	30,433	46,215	3,261	5,844	3,553	6,701	3,993	100,00
KAXXAI05	*k*	20	28	2	4	2	4	2	62
	d_{min}	0,922	1,361	0,869	1,366	0,818	1,226	1,758	0,82
	d_{max}	1,011	1,518	0,869	1,410	0,818	1,320	1,758	1,76
	S	118,955	182,324	12,268	22,713	14,529	25,897	16,095	392,78
	V	18,519	42,308	1,777	5,246	1,981	5,488	4,717	80,04
	Δ_S	30,285	46,419	3,123	5,783	3,699	6,593	4,098	100,00
KAXXAI06	*k*	20	28	2	4	2	4	2	62
	d_{min}	0,945	1,400	0,951	1,428	0,951	1,237	1,742	0,95
	d_{max}	0,971	1,532	0,951	1,429	0,951	1,335	1,742	1,74
	S	113,439	187,283	12,689	22,381	15,119	27,947	14,977	393,84
	V	18,016	44,866	2,012	5,327	2,397	5,983	4,349	82,95
	Δ_S	28,804	47,554	3,222	5,683	3,839	7,096	3,803	100,00
KAXXAI11	*k*	20	28	2	4	2	4	2	62
	d_{min}	0,960	1,503	0,843	1,419	0,842	1,314	1,743	0,84
	d_{max}	0,960	1,503	0,843	1,419	0,842	1,314	1,743	1,74
	S	118,591	183,335	12,353	22,267	15,467	26,560	14,426	393,00
	V	18,474	42,702	1,735	5,180	2,170	5,634	4,190	80,09
	Δ_S	30,176	46,650	3,143	5,666	3,936	6,758	3,671	100,00

Table S13. Characteristics of chemical bonds in *N*-(3-chloro-2-methylphenyl)anthranilic acid (**III**) polymorphs (VD polyhedra faces with RF > 1)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	H/Cl	C/Cl	N/Cl	O/Cl	Cl/Cl	∑
KAXXAI09	k	26	62	18	6			6	2			6	2				128
	d_{min}	1,686	1,924	2,386	2,452			1,852	2,355			2,786	3,046				1,69
	d_{max}	3,697	3,494	2,789	2,614			2,334	2,355			2,993	3,046				3,70
	S	53,236	43,046	1,422	9,155			21,254	0,156			13,340	0,087				141,70
	V	20,717	17,358	0,586	3,837			7,361	0,061			6,417	0,044				56,38
	Δ_S	37,571	30,379	1,004	6,461			15,000	0,110			9,415	0,061				100,00
KAXXAI10	k	22	58	20	6	2		10	2			6	2				128
	d_{min}	1,686	1,916	2,382	2,511	2,400		1,800	2,352			2,651	3,028				1,69
	d_{max}	2,764	3,001	2,782	2,675	2,400		3,748	2,352			3,271	3,028				3,75
	S	55,934	34,617	1,500	6,508	0,007		27,584	0,232			13,805	0,070				140,26
	V	20,599	13,559	0,612	2,824	0,003		9,909	0,091			6,398	0,035				54,03
	Δ_S	39,880	24,681	1,069	4,640	0,005		19,667	0,165			9,843	0,050				100,00
KAXXAI02	k	23	61	18	6	2		8	3			5					126
	d_{min}	1,567	1,764	2,378	2,507	2,400		1,907	2,350			2,582					1,57
	d_{max}	4,166	4,083	2,781	2,620	2,801		3,530	2,386			3,366					4,17
	S	64,512	40,335	1,133	8,421	0,025		26,518	0,157			15,276					156,38
	V	23,044	15,291	0,459	3,632	0,010		9,879	0,062			6,936					59,31
	Δ_S	41,254	25,793	0,725	5,385	0,016		16,958	0,100			9,769					100,00
Mol A	k	22	58	22	6			6	2			6					122
	d_{min}	1,568	1,764	2,378	2,507			2,000	2,350			2,653					1,57
	d_{max}	2,695	2,979	2,781	2,606			2,362	2,350			3,366					3,37
	S	66,376	40,341	1,283	7,692			24,902	0,139			15,451					156,18
	V	23,523	15,326	0,523	3,286			9,006	0,055			7,122					58,84
	Δ_S	42,499	25,829	0,821	4,925			15,944	0,089			9,893					100,00

Table S13 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	H/Cl	C/Cl	N/Cl	O/Cl	Cl/Cl	∑
Mol B	k	24	64	14	6	4		10	4			4					130
	d_{min}	1,567	1,771	2,386	2,594	2,400		1,907	2,360			2,582					1,57
	d_{max}	4,166	4,083	2,779	2,620	2,801		3,530	2,386			2,772					4,17
	S	62,648	40,329	0,983	9,150	0,051		28,135	0,174			15,101					156,57
	V	22,564	15,256	0,395	3,978	0,021		10,753	0,069			6,750					59,79
	Δ_S	40,013	25,758	0,628	5,844	0,033		17,969	0,111			9,645					100,00
KAXXAI03	k	23	62	19	6	1		7	2			6	1				127
	d_{min}	1,600	1,727	2,370	2,444	2,418		1,903	2,340			2,664	3,016				1,60
	d_{max}	4,012	3,874	2,782	2,616	2,418		3,399	2,355			3,370	3,043				4,01
	S	64,770	42,053	1,186	8,692	0,005		25,609	0,181			14,994	0,022				157,51
	V	23,763	16,079	0,479	3,685	0,002		9,176	0,071			7,025	0,011				60,29
	Δ_S	41,120	26,698	0,753	5,518	0,003		16,258	0,115			9,519	0,014				100,00
Mol A	k	24	64	18	6			8	2			6	2				130
	d_{min}	1,600	1,784	2,370	2,444			1,903	2,355			2,770	3,016				1,60
	d_{max}	4,012	3,874	2,774	2,607			3,399	2,355			3,050	3,016				4,01
	S	61,178	43,728	1,150	8,338			26,719	0,100			16,289	0,048				157,55
	V	22,281	16,935	0,462	3,540			9,648	0,039			7,702	0,024				60,63
	Δ_S	38,831	27,755	0,730	5,292			16,959	0,063			10,339	0,030				100,00
Mol B	k	24	62	20	6	2		6	2			6	2				130
	d_{min}	1,600	1,782	2,371	2,465	2,418		1,906	2,354			2,699	3,043				1,60
	d_{max}	3,964	3,571	2,782	2,616	2,418		2,383	2,354			3,200	3,043				3,96
	S	64,581	42,444	1,186	9,053	0,014		23,449	0,140			14,233	0,018				155,12
	V	24,058	16,181	0,476	3,830	0,006		8,308	0,055			6,692	0,009				59,62
	Δ_S	41,633	27,362	0,765	5,836	0,009		15,117	0,090			9,176	0,012				100,00

Table S13 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	H/Cl	C/Cl	N/Cl	O/Cl	Cl/Cl	∑
Mol C	k	22	60	18	6			6	2			6					120
	d_{min}	1,600	1,727	2,376	2,493			2,006	2,340			2,664					1,60
	d_{max}	2,848	3,457	2,779	2,598			2,352	2,340			3,370					3,46
	S	68,551	39,986	1,222	8,687			26,661	0,303			14,461					159,87
	V	24,950	15,121	0,500	3,685			9,571	0,118			6,680					60,63
	Δ_S	42,879	25,011	0,764	5,434			16,677	0,190			9,045					100,00
KAXXAI04	k	26	65	24	7	3		6	2		2	6	2				143
	d_{min}	1,567	1,738	2,360	1,606	2,173		1,929	2,337		2,216	2,683	3,040				1,57
	d_{max}	3,754	3,873	3,113	3,289	2,264		2,404	2,348		2,222	3,231	3,045				3,87
	S	60,040	44,656	3,748	7,824	1,474		25,652	0,306		0,115	15,965	0,021				159,80
	V	21,509	17,085	1,589	2,366	0,542		9,282	0,120		0,042	7,559	0,011				60,10
	Δ_S	37,572	27,945	2,345	4,896	0,922		16,052	0,191		0,072	9,991	0,013				100,00
KAXXAI07	k	24	62	18	6	2		6	2			6					126
	d_{min}	1,567	1,768	2,356	2,579	2,426		1,962	2,355			2,633					1,57
	d_{max}	3,974	3,413	2,776	2,610	2,426		2,377	2,355			3,467					3,97
	S	73,066	43,049	1,497	8,627	0,021		25,753	0,140			18,200					170,35
	V	26,470	16,363	0,596	3,721	0,008		9,229	0,055			8,244					64,69
	Δ_S	42,891	25,270	0,879	5,064	0,012		15,117	0,082			10,684					100,00
KAXXAI05	k	24	60	16	6	2		8	2			6					124
	d_{min}	1,566	1,784	2,344	2,592	2,392		1,958	2,342			2,502					1,57
	d_{max}	4,043	3,448	2,757	2,635	2,392		3,850	2,342			3,427					4,04
	S	77,033	42,790	1,244	8,630	0,026		26,507	0,279			21,341					177,85
	V	27,532	16,312	0,491	3,758	0,010		9,529	0,109			9,426					67,17
	Δ_S	43,314	24,060	0,699	4,852	0,015		14,904	0,157			12,000					100,00

Table S13 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	H/Cl	C/Cl	N/Cl	O/Cl	Cl/Cl	∑
KAXXAI06	k	24	68	34	8	2		6	2			6					150
	d_{min}	1,540	1,924	2,448	2,535	2,906		1,873	2,403			2,600					1,54
	d_{max}	3,648	3,482	2,865	3,231	2,906		2,597	2,403			3,341					3,65
	S	61,310	42,931	1,460	8,116	0,016		21,136	0,035			13,636					148,64
	V	22,181	16,955	0,614	3,498	0,008		7,596	0,014			6,267					57,13
	Δ_S	41,248	28,883	0,982	5,460	0,011		14,220	0,024			9,174					100,00
KAXXAI11	k	22	58	14	6			8	2			6	2				118
	d_{min}	1,568	1,784	2,365	2,446			1,990	2,336			2,721	3,050				1,57
	d_{max}	2,969	2,932	2,753	2,609			3,528	2,336			3,191	3,050				3,53
	S	68,437	39,310	1,331	7,155			26,119	0,276			12,857	0,010				155,50
	V	24,370	14,750	0,550	3,027			9,575	0,108			5,978	0,005				58,36
	Δ_S	44,012	25,280	0,856	4,601			16,797	0,177			8,268	0,006				100,00

Table S14. Characteristics of chemical bonds in *N*-(3-chloro-2-methylphenyl)anthranilic acid (**III**) polymorphs (VD polyhedra faces with RF = 0)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	H/Cl	C/Cl	N/Cl	O/Cl	Cl/Cl	∑
KAXXAI09	k	65	102	21	4	2		18	20	2	2	24	6			2	268
	d_{min}	2,126	2,633	3,439	3,507	3,977		1,626	3,321	3,729	3,518	2,809	3,567			4,061	1,63
	d_{max}	3,991	4,292	3,807	3,584	3,977		3,821	3,840	3,729	3,518	4,472	4,193			4,061	4,47
	S	132,512	71,345	10,349	0,843	0,003		34,321	12,833	0,368	1,174	47,587	6,298			0,431	318,06
	V	61,765	38,380	6,156	0,493	0,002		14,319	7,513	0,229	0,688	25,977	3,877			0,291	159,69
	Δ_S	41,662	22,431	3,254	0,265	0,001		10,791	4,035	0,116	0,369	14,962	1,980			0,136	100,00
KAXXAI10	k	77	66	78	6	8	2	24	14	2	7	18	8			2	312
	d_{min}	2,304	2,866	3,491	3,135	3,787	3,846	1,640	3,580	3,829	3,796	2,835	3,422			3,846	1,64
	d_{max}	4,599	3,942	3,986	3,685	3,958	3,846	4,805	3,973	3,829	3,875	4,251	3,755			3,846	4,81
	S	143,933	36,410	33,728	2,074	1,627	0,717	40,442	5,445	0,190	1,910	36,086	8,318			1,590	312,47
	V	65,255	20,928	20,508	1,261	1,051	0,459	18,439	3,349	0,121	1,225	18,432	4,935			1,020	156,98
	Δ_S	46,063	11,652	10,794	0,664	0,521	0,229	12,943	1,743	0,061	0,611	11,549	2,662			0,509	100,00
KAXXAI02	k	79	91	21	5			23	19	1		22	10	1		1	273
	d_{min}	2,489	2,846	3,327	3,072			1,791	3,210	3,886		3,070	3,436	4,181		3,376	1,79
	d_{max}	4,377	4,399	4,121	3,765			4,167	3,770	3,886		4,353	4,345	4,181		3,376	4,40
	S	123,995	78,382	9,162	2,699			39,792	9,698	0,046		37,062	8,161	0,015		5,755	314,77
	V	62,494	42,201	5,310	1,611			17,929	5,534	0,030		21,952	4,960	0,011		3,238	165,27
	Δ_S	39,393	24,902	2,911	0,857			12,642	3,081	0,015		11,774	2,593	0,005		1,828	100,00
Mol A	k	80	88	21	5			23	20			25	10	1		1	274
	d_{min}	2,511	2,846	3,327	3,284			1,791	3,210			3,350	3,436	4,181		3,376	1,79
	d_{max}	4,377	4,399	4,121	3,765			4,167	3,770			4,214	4,346	4,181		3,376	4,40
	S	122,111	78,638	8,958	3,179			42,021	9,092			38,637	8,161	0,016		5,755	316,57
	V	61,800	42,410	5,200	1,914			18,952	5,231			23,453	4,960	0,011		3,239	167,17
	Δ_S	38,574	24,841	2,830	1,004			13,274	2,872			12,205	2,578	0,005		1,818	100,00

Table S14 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	H/Cl	C/Cl	N/Cl	O/Cl	Cl/Cl	∑
Mol B	k	78	94	21	5			23	18	2		19	10	1		1	272
	d_{min}	2,489	2,863	3,360	3,072			1,791	3,210	3,886		3,070	3,436	4,181		3,376	1,79
	d_{max}	4,377	4,399	4,121	3,603			4,167	3,770	3,886		4,353	4,346	4,181		3,376	4,40
	S	125,880	78,128	9,366	2,220			37,563	10,304	0,092		35,489	8,161	0,016		5,755	312,97
	V	63,188	41,991	5,421	1,308			16,907	5,838	0,059		20,452	4,960	0,011		3,239	163,37
	Δ_S	40,221	24,963	2,992	0,709			12,002	3,292	0,029		11,339	2,608	0,005		1,839	100,00
KAXXAI03	k	79	97	20	5			23	16	1		20	13	1		1	276
	d_{min}	2,407	2,649	3,359	3,027			1,773	3,203	3,799		2,948	3,537	3,953		3,412	1,77
	d_{max}	4,488	4,503	4,274	3,711			4,219	3,863	3,967		4,439	4,223	3,953		3,530	4,50
	S	123,084	81,431	7,323	2,363			40,613	9,966	0,031		38,334	7,561	0,133		4,504	315,34
	V	62,471	43,308	4,277	1,380			18,299	5,712	0,020		21,351	4,712	0,087		2,612	164,23
	Δ_S	39,032	25,823	2,322	0,749			12,879	3,160	0,010		12,156	2,398	0,042		1,428	100,00
Mol A	k	77	98	17	5			24	17	1		16	15			1	271
	d_{min}	2,457	2,649	3,359	3,075			1,773	3,203	3,967		2,948	3,627			3,530	1,77
	d_{max}	4,384	4,503	4,274	3,707			4,219	3,863	3,967		4,288	4,223			3,530	4,50
	S	133,170	77,814	7,880	3,264			38,758	10,341	0,028		31,898	9,529			3,885	316,56
	V	67,480	41,678	4,598	1,855			17,724	5,931	0,019		17,734	5,974			2,286	165,28
	Δ_S	42,067	24,581	2,489	1,031			12,243	3,266	0,009		10,076	3,010			1,227	100,00
Mol B	k	80	86	26	6			22	16	2		19	15			1	273
	d_{min}	2,407	2,872	3,411	3,027			1,793	3,203	3,799		2,948	3,627			3,530	1,79
	d_{max}	4,488	4,503	4,163	3,711			4,219	3,825	3,799		4,439	4,223			3,530	4,50
	S	122,322	78,367	8,128	1,587			41,109	10,089	0,038		38,691	9,529			3,885	313,74
	V	61,789	41,596	4,780	0,947			17,943	5,730	0,024		21,309	5,974			2,286	162,38
	Δ_S	38,988	24,978	2,591	0,506			13,103	3,216	0,012		12,332	3,037			1,238	100,00

Table S14 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	H/Cl	C/Cl	N/Cl	O/Cl	Cl/Cl	∑
Mol C	k	81	106	16	5			24	15	1		25	8	2		1	284
	d_{min}	2,407	2,649	3,359	3,182			1,793	3,403	3,967		3,028	3,537	3,953		3,412	1,79
	d_{max}	4,488	4,355	4,274	3,711			4,041	3,863	3,967		4,400	4,052	3,953		3,412	4,49
	S	113,760	88,113	5,963	2,238			41,974	9,468	0,028		44,412	3,625	0,398		5,741	315,72
	V	58,143	46,649	3,454	1,337			19,231	5,475	0,019		25,011	2,190	0,262		3,265	165,03
	Δ_S	36,032	27,909	1,889	0,709			13,295	2,999	0,009		14,067	1,148	0,126		1,818	100,00
KAXXAI04	k	74,5	83	35,5	4	1		27	6			18	9		6	1	265
	d_{min}	2,248	2,717	3,453	3,349	3,797		1,687	3,431			2,785	3,904		3,437	2,869	1,69
	d_{max}	4,279	4,241	3,986	4,115	3,797		4,447	4,088			4,635	4,546		4,111	4,137	4,64
	S	128,972	72,076	15,521	0,373	0,036		43,046	2,683			34,568	4,393		9,201	3,134	314,00
	V	66,152	38,485	9,310	0,249	0,023		19,906	1,604			19,212	2,949		5,503	1,532	164,92
	Δ_S	41,074	22,954	4,943	0,119	0,011		13,709	0,854			11,009	1,399		2,930	0,998	100,00
KAXXAI07	k	83	88	20	4			24	20	2		26	12			1	280
	d_{min}	2,522	2,807	3,451	3,119			1,828	3,380	3,863		3,200	3,372			3,352	1,83
	d_{max}	4,499	4,430	4,219	3,664			3,993	4,053	3,863		4,674	4,365			3,352	4,67
	S	126,334	80,276	7,363	1,892			40,250	10,062	0,005		34,976	7,478			8,331	316,97
	V	64,190	42,246	4,322	1,123			18,247	5,793	0,003		21,068	4,413			4,655	166,06
	Δ_S	39,857	25,326	2,323	0,597			12,699	3,174	0,002		11,035	2,359			2,628	100,00
KAXXAI05	k	83	80	13	4			24	20	2		28	12			2	268
	d_{min}	2,588	2,942	3,481	3,255			1,840	3,400	3,952		3,434	3,363			3,838	1,84
	d_{max}	4,462	4,458	3,890	3,762			4,174	3,988	3,952		4,904	4,374			3,838	4,90
	S	134,452	76,618	5,649	2,648			40,152	10,581	0,011		36,285	13,654			4,773	324,82
	V	68,642	42,045	3,327	1,605			18,475	6,166	0,007		23,166	8,140			3,053	174,63
	Δ_S	41,393	23,588	1,739	0,815			12,361	3,257	0,003		11,171	4,204			1,469	100,00

Table S14 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	H/Cl	C/Cl	N/Cl	O/Cl	Cl/Cl	∑
KAXXAI06	k	69	100	29	4			20	16	2	2	24	8			2	276
	d_{min}	2,183	2,572	3,440	3,476			1,694	3,435	3,817	3,483	3,116	3,668			4,019	1,69
	d_{max}	4,192	4,398	4,001	3,534			4,063	3,820	3,817	3,483	4,543	4,387			4,074	4,54
	S	126,417	73,768	13,121	1,357			35,657	11,293	0,028	2,441	49,911	4,276			1,893	320,16
	V	59,300	40,655	7,880	0,797			15,170	6,678	0,018	1,417	28,487	2,706			1,273	164,38
	Δ_S	39,486	23,041	4,098	0,424			11,137	3,527	0,009	0,762	15,589	1,336			0,591	100,00
KAXXAI11	k	70	106	29	10	4		26	14			18	14		2	1	294
	d_{min}	2,441	2,953	3,442	3,234	3,802		1,825	3,582			2,824	3,592		3,536	3,896	1,83
	d_{max}	4,400	4,324	4,082	3,965	3,843		4,387	4,515			4,244	4,049		3,536	3,896	4,52
	S	117,899	84,020	7,584	2,136	1,762		43,592	6,414			39,706	7,606		5,375	0,943	317,04
	V	58,972	46,870	4,534	1,239	1,125		20,344	3,949			20,924	4,675		3,168	0,612	166,41
	Δ_S	37,188	26,502	2,392	0,674	0,556		13,750	2,023			12,524	2,399		1,695	0,297	100,00

Table S15. Characteristics of chemical bonds in 2-(methylphenylamino)nicotinic acid (**IV**) polymorphs (VD polyhedra faces with RF = 1)

		H/C	C/C	C/N	H/O	C/O	∑
MOTNUF	*k*	22	22	10	2	4	60
	d_{min}	0,950	1,370	1,345	0,840	1,199	0,84
	d_{max}	0,981	1,495	1,456	0,840	1,360	1,50
	S	133,075	141,503	51,125	13,689	25,040	364,43
	V	21,162	32,985	11,788	1,916	5,294	73,15
	Δ_S	36,516	38,828	14,029	3,756	6,871	100,00
MOTNUF01	*k*	22	22	10	2	4	60
	d_{min}	0,949	1,358	1,337	0,840	1,204	0,84
	d_{max}	0,982	1,496	1,474	0,841	1,335	1,50
	S	131,429	149,921	55,694	13,706	25,194	375,94
	V	20,900	34,855	12,827	1,919	5,304	75,81
	Δ_S	34,960	39,878	14,814	3,646	6,702	100,00
Mol A	*k*	22	22	10	2	4	60
	d_{min}	0,949	1,368	1,337	0,841	1,215	0,84
	d_{max}	0,982	1,496	1,465	0,841	1,335	1,50
	S	131,530	148,141	55,658	13,230	25,141	373,70
	V	20,917	34,442	12,778	1,854	5,307	75,30
	Δ_S	35,197	39,642	14,894	3,540	6,728	100,00
Mol B	*k*	22	22	10	2	4	60
	d_{min}	0,949	1,359	1,342	0,840	1,204	0,84
	d_{max}	0,981	1,494	1,468	0,840	1,325	1,49
	S	132,114	152,049	53,359	12,798	25,653	375,97
	V	21,003	35,353	12,303	1,791	5,382	75,83
	Δ_S	35,139	40,441	14,192	3,404	6,823	100,00
Mol C	*k*	22	22	10	2	4	60
	d_{min}	0,949	1,358	1,351	0,840	1,215	0,84
	d_{max}	0,981	1,489	1,474	0,840	1,329	1,49
	S	130,643	149,574	58,066	15,090	24,788	378,16
	V	20,780	34,771	13,400	2,113	5,224	76,29
	Δ_S	34,547	39,553	15,355	3,990	6,555	100,00
MOTNUF02	*k*	22	22	10	2	4	60
	d_{min}	0,949	1,359	1,340	0,839	1,201	0,84
	d_{max}	0,981	1,499	1,476	0,966	1,336	1,50
	S	130,261	149,478	54,969	14,354	25,621	374,68
	V	20,719	34,798	12,685	2,105	5,395	75,70
	Δ_S	34,766	39,895	14,671	3,831	6,838	100,00
Mol A	*k*	22	22	10	2	4	60
	d_{min}	0,949	1,359	1,355	0,966	1,220	0,95
	d_{max}	0,981	1,490	1,473	0,966	1,328	1,49
	S	131,425	146,392	53,398	13,752	24,316	369,28
	V	20,900	34,015	12,349	2,214	5,140	74,62
	Δ_S	35,589	39,642	14,460	3,724	6,585	100,00

Table S15 (continued)

		H/C	C/C	C/N	H/O	C/O	∑
Mol B	*k*	22	22	10	2	4	60
	d_{min}	0,950	1,369	1,344	0,840	1,207	0,84
	d_{max}	0,980	1,497	1,470	0,840	1,334	1,50
	S	128,707	144,569	57,148	16,251	25,208	371,88
	V	20,474	33,665	13,189	2,276	5,307	74,91
	Δ_S	34,610	38,875	15,367	4,370	6,778	100,00
Mol C	*k*	22	22	10	2	4	60
	d_{min}	0,949	1,368	1,340	0,839	1,201	0,84
	d_{max}	0,980	1,499	1,476	0,839	1,336	1,50
	S	130,652	157,471	54,361	13,059	27,341	382,88
	V	20,783	36,713	12,517	1,826	5,738	77,58
	Δ_S	34,123	41,128	14,198	3,411	7,141	100,00
MOTNUF03	*k*	22	22	10	2	4	60
	d_{min}	0,948	1,352	1,324	0,840	1,195	0,84
	d_{max}	0,982	1,499	1,471	0,841	1,339	1,50
	S	130,767	145,074	53,479	13,819	23,984	367,12
	V	20,797	33,649	12,255	1,935	5,030	73,67
	Δ_S	35,619	39,517	14,567	3,764	6,533	100,00
Mol A	*k*	22	22	10	2	4	60
	d_{min}	0,949	1,365	1,324	0,840	1,214	0,84
	d_{max}	0,980	1,475	1,459	0,840	1,333	1,48
	S	126,933	141,138	55,774	16,204	24,657	364,71
	V	20,195	32,754	12,756	2,268	5,205	73,18
	Δ_S	34,804	38,699	15,293	4,443	6,761	100,00
Mol B	*k*	22	22	10	2	4	60
	d_{min}	0,950	1,372	1,340	0,841	1,202	0,84
	d_{max}	0,980	1,492	1,450	0,841	1,324	1,49
	S	127,344	142,138	55,540	16,131	25,057	366,21
	V	20,268	32,978	12,719	2,260	5,246	73,47
	Δ_S	34,773	38,813	15,166	4,405	6,842	100,00
Mol C	*k*	22	22	10	2	4	60
	d_{min}	0,949	1,367	1,332	0,840	1,208	0,84
	d_{max}	0,981	1,483	1,471	0,840	1,323	1,48
	S	133,710	148,114	52,595	13,767	22,272	370,46
	V	21,261	34,324	12,083	1,927	4,669	74,26
	Δ_S	36,093	39,981	14,197	3,716	6,012	100,00
Mol D	*k*	22	22	10	2	4	60
	d_{min}	0,948	1,366	1,328	0,840	1,210	0,84
	d_{max}	0,981	1,486	1,465	0,840	1,317	1,49
	S	131,604	142,198	53,868	13,261	22,533	363,46
	V	20,929	33,020	12,322	1,857	4,718	72,85
	Δ_S	36,208	39,123	14,821	3,649	6,200	100,00

Table S15 (continued)

		H/C	C/C	C/N	H/O	C/O	∑
Mol E	k	22	22	10	2	4	60
	d_{min}	0,949	1,367	1,341	0,841	1,203	0,84
	d_{max}	0,982	1,483	1,459	0,841	1,339	1,48
	S	131,740	142,751	53,990	13,653	22,793	364,93
	V	20,949	33,087	12,385	1,913	4,796	73,13
	Δ_S	36,100	39,118	14,795	3,741	6,246	100,00
Mol F	k	22	22	10	2	4	60
	d_{min}	0,949	1,352	1,332	0,840	1,213	0,84
	d_{max}	0,981	1,482	1,456	0,840	1,317	1,48
	S	132,929	148,743	52,886	13,977	22,353	370,89
	V	21,140	34,452	12,120	1,957	4,689	74,36
	Δ_S	35,841	40,105	14,259	3,769	6,027	100,00
Mol G	k	22	22	10	2	4	60
	d_{min}	0,948	1,373	1,335	0,841	1,206	0,84
	d_{max}	0,979	1,477	1,469	0,841	1,330	1,48
	S	128,482	140,230	52,533	12,975	24,496	358,72
	V	20,429	32,623	12,050	1,818	5,145	72,07
	Δ_S	35,817	39,092	14,645	3,617	6,829	100,00
Mol H	k	22	22	10	2	4	60
	d_{min}	0,949	1,374	1,334	0,840	1,210	0,84
	d_{max}	0,980	1,484	1,471	0,840	1,323	1,48
	S	128,349	140,145	52,531	13,122	24,570	358,72
	V	20,413	32,584	12,049	1,836	5,159	72,04
	Δ_S	35,780	39,068	14,644	3,658	6,849	100,00
Mol I	k	22	22	10	2	4	60
	d_{min}	0,949	1,354	1,329	0,840	1,200	0,84
	d_{max}	0,980	1,473	1,453	0,840	1,328	1,47
	S	133,143	152,228	52,541	12,611	25,441	375,96
	V	21,172	35,235	12,025	1,766	5,326	75,52
	Δ_S	35,414	40,490	13,975	3,354	6,767	100,00
Mol J	k	22	22	10	2	4	60
	d_{min}	0,948	1,355	1,333	0,840	1,195	0,84
	d_{max}	0,980	1,499	1,463	0,840	1,321	1,50
	S	133,433	153,057	52,530	12,485	25,666	377,17
	V	21,213	35,438	12,039	1,748	5,349	75,79
	Δ_S	35,377	40,580	13,927	3,310	6,805	100,00

Table S16. Characteristics of chemical bonds in 2-(methylphenylamino)nicotinic acid (**IV**) polymorphs (VD polyhedra faces with RF > 1)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
MOTNUF	*k*	22	48	36	16	6	2	8	16	2		156
	d_{min}	1,600	1,821	2,322	1,977	2,463	2,316	2,313	2,343	3,061		1,60
	d_{max}	3,438	3,405	3,185	2,875	3,001	2,316	3,649	3,861	3,061		3,86
	S	64,373	24,852	5,889	19,870	0,457	0,272	16,863	10,091	2,341		145,01
	V	23,693	10,618	2,840	7,576	0,214	0,105	7,564	4,799	1,194		58,60
	Δ_S	44,392	17,138	4,061	13,703	0,315	0,188	11,629	6,959	1,614		100,00
MOTNUF01	*k*	23	53	38	17	7	2	9	17	2		168
	d_{min}	1,600	1,789	2,318	1,976	2,400	2,313	2,294	2,323	2,977		1,60
	d_{max}	4,089	4,300	3,136	3,679	3,024	2,314	4,148	4,343	3,098		4,34
	S	59,769	27,149	5,628	17,271	0,438	0,294	14,799	11,244	1,611		138,20
	V	21,490	11,775	2,664	6,634	0,199	0,113	6,516	5,411	0,813		55,62
	Δ_S	43,248	19,644	4,072	12,497	0,317	0,213	10,708	8,136	1,166		100,00
Mol A	*k*	24	52	38	16	8	2	10	16	2		168
	d_{min}	1,601	1,799	2,319	1,976	2,401	2,314	2,313	2,340	3,098		1,60
	d_{max}	4,084	3,914	3,117	2,756	3,024	2,314	4,036	3,850	3,098		4,08
	S	56,876	24,452	6,051	16,840	0,494	0,186	12,489	11,101	1,080		129,57
	V	20,660	10,359	2,862	6,448	0,221	0,072	5,569	5,328	0,557		52,08
	Δ_S	43,896	18,872	4,670	12,997	0,381	0,144	9,639	8,568	0,834		100,00
Mol B	*k*	20	54	40	18	8	2	8	18	2		170
	d_{min}	1,600	1,789	2,318	1,977	2,400	2,313	2,294	2,323	2,977		1,60
	d_{max}	2,352	4,300	3,136	3,544	3,016	2,313	3,609	4,343	2,977		4,34
	S	68,615	27,623	5,049	16,412	0,370	0,509	14,847	11,142	2,408		146,98
	V	24,050	12,118	2,397	6,183	0,171	0,196	6,184	5,532	1,194		58,03
	Δ_S	46,685	18,794	3,435	11,167	0,252	0,346	10,102	7,581	1,638		100,00

Table S16 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
Mol C	*k*	24	54	36	18	6	2	10	18	2		170
	d_{min}	1,600	1,794	2,320	1,986	2,453	2,314	2,302	2,340	3,067		1,60
	d_{max}	4,089	3,897	3,120	3,679	3,016	2,314	4,148	3,938	3,067		4,15
	S	53,815	29,373	5,783	18,560	0,449	0,186	17,062	11,488	1,346		138,06
	V	19,758	12,849	2,732	7,271	0,204	0,072	7,797	5,374	0,688		56,75
	Δ_S	38,979	21,275	4,189	13,443	0,325	0,135	12,358	8,321	0,975		100,00
MOTNUF02	*k*	24	55	35	17	7	2	9	16	2		167
	d_{min}	1,600	1,798	2,306	1,972	2,410	2,318	2,305	2,332	2,944		1,60
	d_{max}	4,377	4,350	3,685	3,566	3,027	2,331	4,291	4,057	3,160		4,38
	S	55,189	26,672	6,142	18,708	0,493	0,223	15,821	11,069	2,536		136,85
	V	19,991	11,714	2,933	7,294	0,225	0,087	7,213	5,248	1,263		55,97
	Δ_S	40,328	19,490	4,488	13,670	0,360	0,163	11,561	8,088	1,853		100,00
Mol A	*k*	26	54	42	16	8	2	10	18	2		178
	d_{min}	1,600	1,942	2,329	1,986	2,410	2,318	2,428	2,342	3,160		1,60
	d_{max}	3,909	3,736	3,685	2,664	3,027	2,318	3,887	3,669	3,160		3,91
	S	53,677	22,162	6,368	16,875	0,389	0,184	12,328	11,896	0,801		124,68
	V	19,641	9,667	3,011	6,487	0,179	0,071	5,680	5,707	0,422		50,87
	Δ_S	43,052	17,775	5,107	13,535	0,312	0,148	9,888	9,541	0,642		100,00
Mol B	*k*	24	56	32	18	6	2	10	16	2		166
	d_{min}	1,600	1,798	2,317	1,986	2,458	2,331	2,307	2,337	3,019		1,60
	d_{max}	4,377	4,143	3,102	3,566	2,999	2,331	4,291	4,057	3,019		4,38
	S	50,734	28,243	5,947	19,950	0,502	0,155	16,790	10,583	2,082		134,99
	V	18,581	12,193	2,821	8,009	0,229	0,060	7,726	5,070	1,048		55,74
	Δ_S	37,585	20,923	4,406	14,779	0,372	0,115	12,438	7,840	1,542		100,00

Table S16 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
Mol C	*k*	22	54	32	18	6	2	8	14	2		158
	d_{min}	1,600	1,800	2,306	1,972	2,439	2,328	2,305	2,332	2,944		1,60
	d_{max}	3,540	4,350	3,349	3,458	2,960	2,328	3,869	3,882	2,944		4,35
	S	61,155	29,611	6,111	19,300	0,588	0,331	18,344	10,727	4,724		150,89
	V	21,750	13,284	2,965	7,386	0,268	0,128	8,233	4,966	2,318		61,30
	Δ_S	40,529	19,624	4,050	12,791	0,390	0,219	12,157	7,109	3,131		100,00
MOTNUF03	*k*	24	53	34	17	7	2	9	17	2	2	167
	d_{min}	1,597	1,782	2,299	1,963	2,382	2,294	2,287	2,303	2,953	2,223	1,60
	d_{max}	4,436	4,299	3,727	3,532	3,000	2,320	4,305	4,360	3,134	2,223	4,44
	S	57,123	27,466	5,752	17,859	0,469	0,227	16,587	11,170	1,601	<0,01	138,26
	V	20,732	11,934	2,727	6,925	0,214	0,087	7,665	5,317	0,808	0,000	56,41
	Δ_S	41,317	19,866	4,160	12,918	0,339	0,164	11,997	8,079	1,158	0,001	100,00
Mol A	*k*	24	48	32	18	8	2	10	14	2		158
	d_{min}	1,599	1,796	2,299	1,978	2,393	2,305	2,287	2,327	3,006		1,60
	d_{max}	4,436	3,611	3,101	3,523	2,976	2,305	4,296	4,050	3,006		4,44
	S	49,392	27,919	6,431	19,409	0,499	0,185	17,172	10,010	2,102		133,12
	V	18,013	12,013	3,021	7,732	0,228	0,071	7,897	4,806	1,053		54,83
	Δ_S	37,104	20,973	4,831	14,580	0,375	0,139	12,900	7,520	1,579		100,00
Mol B	*k*	24	52	34	18	6	2	10	16	2		164
	d_{min}	1,599	1,789	2,307	1,976	2,443	2,304	2,307	2,332	3,007		1,60
	d_{max}	4,338	4,097	3,121	3,525	3,000	2,304	4,305	4,062	3,007		4,34
	S	50,749	27,540	5,948	19,880	0,429	0,200	17,096	10,216	2,102		134,16
	V	18,659	11,896	2,826	7,935	0,194	0,077	7,810	4,868	1,053		55,32
	Δ_S	37,827	20,528	4,434	14,818	0,320	0,149	12,743	7,615	1,567		100,00

Table S16 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
Mol C	*k*	26	52	34	16	8	2	10	18	2		168
	d_{min}	1,601	1,788	2,313	1,981	2,382	2,294	2,294	2,334	3,125		1,60
	d_{max}	3,960	3,751	3,183	2,632	3,000	2,294	4,013	3,783	3,125		4,01
	S	56,556	29,376	5,701	18,204	0,479	0,187	18,082	11,922	1,033		141,54
	V	20,729	12,993	2,692	7,044	0,219	0,072	8,762	5,544	0,538		58,59
	Δ_S	39,958	20,755	4,028	12,861	0,338	0,132	12,775	8,423	0,730		100,00
Mol D	*k*	26	54	28	16	8	2	10	18	2		164
	d_{min}	1,599	1,783	2,302	1,963	2,393	2,317	2,308	2,326	3,134		1,60
	d_{max}	3,888	3,701	3,210	2,690	3,000	2,317	3,984	3,750	3,134		3,98
	S	58,832	28,659	6,325	18,580	0,473	0,099	18,837	12,286	0,863		144,95
	V	21,854	12,730	2,981	7,193	0,215	0,038	9,106	5,648	0,451		60,22
	Δ_S	40,587	19,771	4,363	12,818	0,326	0,068	12,995	8,476	0,595		100,00
Mol E	*k*	26	52	38	16	6	2	10	18	2		170
	d_{min}	1,601	1,802	2,313	1,975	2,452	2,304	2,293	2,336	3,133		1,60
	d_{max}	4,051	3,837	3,727	2,688	2,982	2,304	3,977	3,744	3,133		4,05
	S	59,220	26,778	6,421	18,549	0,436	0,183	19,157	13,280	0,821		144,85
	V	21,798	11,824	3,026	7,155	0,203	0,070	9,298	6,246	0,429		60,05
	Δ_S	40,885	18,487	4,433	12,806	0,301	0,126	13,226	9,168	0,567		100,00
Mol F	*k*	26	54	36	16	6	2	10	18	2		170
	d_{min}	1,599	1,782	2,299	1,971	2,459	2,300	2,301	2,322	3,112		1,60
	d_{max}	4,045	3,851	3,197	2,689	2,998	2,300	3,987	3,773	3,112		4,05
	S	56,171	28,463	5,859	17,803	0,415	0,227	18,245	12,752	0,929		140,86
	V	20,338	12,450	2,764	6,844	0,192	0,087	8,895	5,960	0,482		58,01
	Δ_S	39,876	20,206	4,159	12,638	0,295	0,161	12,952	9,053	0,660		100,00

Table S16 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
Mol G	*k*	22	54	36	16	8	2	8	14	2		162
	d_{min}	1,598	1,794	2,308	1,972	2,416	2,320	2,293	2,322	3,021		1,60
	d_{max}	3,534	3,607	3,092	2,716	2,983	2,320	3,490	4,010	3,021		4,01
	S	56,027	24,955	5,841	17,328	0,536	0,118	13,348	9,591	2,119		129,86
	V	20,610	10,463	2,779	6,664	0,243	0,046	5,912	4,614	1,067		52,40
	Δ_S	43,143	19,216	4,498	13,343	0,413	0,091	10,279	7,385	1,632		100,00
Mol H	*k*	22	52	34	16	8	2	8	14	2		158
	d_{min}	1,597	1,787	2,318	1,981	2,390	2,301	2,291	2,324	3,033		1,60
	d_{max}	3,545	3,619	3,104	2,673	2,994	2,301	3,514	4,005	3,033		4,01
	S	55,831	24,166	5,707	17,308	0,504	0,138	13,054	9,673	1,905		128,29
	V	20,542	10,142	2,743	6,662	0,228	0,053	5,731	4,677	0,963		51,74
	Δ_S	43,521	18,838	4,449	13,492	0,393	0,108	10,176	7,540	1,485		100,00
Mol I	*k*	20	54	32	18	6	2	8	18	2		160
	d_{min}	1,600	1,793	2,303	1,965	2,455	2,306	2,296	2,303	2,964		1,60
	d_{max}	2,337	4,288	3,133	3,532	2,985	2,306	3,559	4,360	2,964		4,36
	S	64,233	28,644	4,635	15,759	0,472	0,442	15,490	10,889	2,069		142,63
	V	22,390	12,496	2,206	6,006	0,217	0,170	6,631	5,364	1,022		56,50
	Δ_S	45,034	20,082	3,250	11,049	0,331	0,310	10,860	7,634	1,451		100,00
Mol J	*k*	20	54	40	18	6	2	8	18	2	2	170
	d_{min}	1,599	1,786	2,300	1,974	2,447	2,305	2,298	2,324	2,953	2,223	1,60
	d_{max}	2,344	4,299	3,133	3,516	2,988	2,305	3,583	4,340	2,953	2,223	4,34
	S	64,218	28,161	4,652	15,765	0,446	0,491	15,392	11,081	2,069	0,001	142,28
	V	22,387	12,338	2,227	6,014	0,204	0,189	6,612	5,446	1,018	0,001	56,44
	Δ_S	45,136	19,793	3,270	11,081	0,313	0,345	10,818	7,788	1,454	0,001	100,00

Table S17. Characteristics of chemical bonds in 2-(methylphenylamino)nicotinic acid (**IV**) polymorphs (VD polyhedra faces with RF = 0)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
MOTNUF	*k*	86	98		14			30	4	2		234
	d_{min}	2,293	2,643		1,866			2,586	3,607	3,536		1,87
	d_{max}	4,613	4,579		3,979			4,123	4,047	3,536		4,61
	S	138,936	83,049		23,152			55,944	2,536	0,377		303,99
	V	70,292	44,111		9,910			28,362	1,571	0,222		154,47
	Δ_S	45,703	27,319		7,616			18,403	0,834	0,124		100,00
MOTNUF01	*k*	80	105	9	16	3		29	7	1	1	251
	d_{min}	2,196	2,482	3,268	1,829	3,375		2,458	3,180	3,614	3,865	1,83
	d_{max}	4,705	4,484	3,850	4,436	4,437		4,356	4,398	3,614	3,865	4,71
	S	143,734	71,342	2,820	23,967	1,341		52,390	3,233	0,082	0,807	299,72
	V	70,449	40,026	1,736	10,307	0,827		25,548	2,104	0,049	0,520	151,57
	Δ_S	47,957	23,803	0,941	7,997	0,447		17,480	1,079	0,027	0,269	100,00
Mol A	*k*	74	101	14	18	3		33	8		2	253
	d_{min}	2,196	2,751	3,268	1,863	3,375		2,523	3,180		3,865	1,86
	d_{max}	4,700	4,382	3,850	4,008	4,092		4,356	4,398		3,865	4,70
	S	131,277	68,878	4,230	24,345	1,425		60,024	3,364		1,211	294,75
	V	63,341	37,927	2,604	10,716	0,807		28,635	2,205		0,780	147,01
	Δ_S	44,538	23,368	1,435	8,259	0,483		20,364	1,141		0,411	100,00
Mol B	*k*	91	110	3	13	4		27	6	2		256
	d_{min}	2,365	2,901	3,268	1,829	3,375		2,458	3,764	3,614		1,83
	d_{max}	4,705	4,484	3,490	4,436	4,437		4,332	4,398	3,614		4,71
	S	157,224	83,170	0,323	20,325	2,012		45,049	4,486	0,245		312,83
	V	80,455	46,893	0,180	8,545	1,241		23,507	2,901	0,148		163,87
	Δ_S	50,258	26,586	0,103	6,497	0,643		14,400	1,434	0,078		100,00

Table S17 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
Mol C	*k*	75	105	11	17	1		28	6		2	245
	d_{min}	2,196	2,482	3,655	1,852	4,437		2,458	3,180		3,865	1,85
	d_{max}	4,705	4,421	3,850	4,436	4,437		4,356	4,238		3,865	4,71
	S	142,700	61,980	3,907	27,233	0,587		52,099	1,849		1,211	291,56
	V	67,553	35,261	2,424	11,662	0,434		24,501	1,207		0,780	143,82
	Δ_S	48,943	21,258	1,340	9,340	0,201		17,869	0,634		0,415	100,00
MOTNUF02	*k*	82	97	12	14	4		27	7	1	1	245
	d_{min}	2,241	2,522	3,482	1,703	3,349		2,438	3,316	3,370	3,690	1,70
	d_{max}	4,679	4,970	4,102	4,515	4,488		4,213	4,619	3,370	3,949	4,97
	S	148,231	65,737	5,284	22,513	1,566		49,401	3,461	0,036	0,706	296,94
	V	72,337	36,101	3,180	9,566	1,060		23,501	2,241	0,020	0,437	148,44
	Δ_S	49,920	22,139	1,780	7,582	0,527		16,637	1,166	0,012	0,238	100,00
Mol A	*k*	79	92	18	15	5		30	9		2	250
	d_{min}	2,241	2,840	3,482	1,703	3,349		2,438	3,316		3,690	1,70
	d_{max}	4,583	4,792	4,102	3,755	4,488		4,213	4,619		3,949	4,79
	S	137,340	59,961	7,926	24,397	1,389		61,975	3,680		1,060	297,73
	V	65,956	32,355	4,771	10,419	0,876		28,738	2,422		0,656	146,19
	Δ_S	46,130	20,140	2,662	8,194	0,467		20,816	1,236		0,356	100,00
Mol B	*k*	72	98	9	15	1		28	5	2	2	232
	d_{min}	2,360	2,522	3,482	1,877	4,469		2,508	3,316	3,370	3,690	1,88
	d_{max}	4,679	4,469	3,790	4,515	4,469		3,943	3,995	3,370	3,949	4,68
	S	146,506	63,825	3,701	25,861	0,960		49,217	1,934	0,109	1,060	293,17
	V	69,811	35,002	2,197	10,973	0,715		23,552	1,219	0,061	0,656	144,19
	Δ_S	49,973	21,770	1,262	8,821	0,327		16,788	0,660	0,037	0,361	100,00

Table S17 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
Mol C	*k*	95	100	9	12	6		22	8			252
	d_{min}	2,360	2,840	3,501	1,923	3,349		2,438	3,610			1,92
	d_{max}	4,679	4,970	4,102	4,515	4,488		4,213	4,619			4,97
	S	160,848	73,428	4,225	17,281	2,349		37,014	4,770			299,91
	V	81,243	40,946	2,574	7,307	1,591		18,212	3,081			154,95
	Δ_S	53,631	24,483	1,409	5,762	0,783		12,341	1,590			100,00
MOTNUF03	*k*	85	97	12	14	1		29	6	1	2	247
	d_{min}	2,208	2,356	3,293	1,794	3,363		2,379	3,334	3,386	3,650	1,79
	d_{max}	4,669	4,682	4,241	4,353	4,358		4,885	5,128	3,608	4,206	5,13
	S	143,014	69,450	3,729	23,831	0,610		51,657	2,810	0,068	0,718	295,89
	V	69,822	37,496	2,234	10,255	0,407		25,198	1,874	0,039	0,441	147,77
	Δ_S	48,334	23,472	1,260	8,054	0,206		17,458	0,950	0,023	0,243	100,00
Mol A	*k*	78	103	8	15	1		27	5	2	3	242
	d_{min}	2,230	2,470	3,416	1,868	4,352		2,467	3,389	3,386	3,654	1,87
	d_{max}	4,669	4,387	3,774	4,353	4,352		3,814	3,913	3,389	4,206	4,67
	S	142,715	65,123	3,562	26,003	0,955		47,764	2,609	0,121	0,841	289,69
	V	67,339	34,840	2,087	11,073	0,693		22,972	1,625	0,069	0,515	141,21
	Δ_S	49,264	22,480	1,230	8,976	0,329		16,488	0,900	0,042	0,290	100,00
Mol B	*k*	76	102	7	15	1		28	5	2	3	239
	d_{min}	2,237	2,470	3,417	1,868	4,358		2,493	3,465	3,386	3,665	1,87
	d_{max}	4,585	4,417	3,809	4,351	4,358		3,804	3,900	3,389	4,200	4,59
	S	142,227	66,330	3,485	25,713	1,009		47,940	2,320	0,121	0,985	290,13
	V	67,041	35,684	2,041	10,924	0,733		23,187	1,458	0,069	0,606	141,74
	Δ_S	49,022	22,862	1,201	8,863	0,348		16,524	0,800	0,042	0,339	100,00

Table S17 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
Mol C	*k*	87	91	19	16			29	6		3	251
	d_{min}	2,272	2,519	3,416	1,842			2,379	3,465		3,665	1,84
	d_{max}	4,466	4,382	4,241	4,025			4,825	4,800		4,200	4,83
	S	145,234	64,320	5,704	24,119			53,353	1,996		0,985	295,71
	V	71,108	34,830	3,454	10,638			25,666	1,474		0,606	147,77
	Δ_S	49,114	21,751	1,929	8,156			18,042	0,675		0,333	100,00
Mol D	*k*	87	89	20	16			28	7		3	250
	d_{min}	2,272	2,519	3,417	1,842			2,379	3,389		3,654	1,84
	d_{max}	4,664	4,307	4,216	3,989			4,885	5,128		4,206	5,13
	S	146,242	63,609	5,769	23,934			55,395	1,903		0,841	297,69
	V	72,053	34,538	3,491	10,517			26,871	1,419		0,515	149,40
	Δ_S	49,125	21,367	1,938	8,040			18,608	0,639		0,283	100,00
Mol E	*k*	91	88	19	16			29	6		3	252
	d_{min}	2,344	2,797	3,414	1,838			2,380	3,334		3,657	1,84
	d_{max}	4,664	4,382	4,241	4,025			4,825	4,800		4,167	4,83
	S	146,011	63,553	5,705	24,086			54,976	1,927		0,902	297,16
	V	71,641	34,605	3,471	10,587			26,646	1,429		0,553	148,93
	Δ_S	49,136	21,387	1,920	8,105			18,500	0,648		0,303	100,00
Mol F	*k*	84	87	20	16			29	7		3	246
	d_{min}	2,344	2,802	3,392	1,838			2,380	3,407		3,650	1,84
	d_{max}	4,474	4,256	4,216	3,989			4,885	5,128		4,137	5,13
	S	145,189	63,962	5,758	24,269			52,909	2,077		0,864	295,03
	V	70,954	34,786	3,495	10,612			25,380	1,524		0,532	147,28
	Δ_S	49,212	21,680	1,952	8,226			17,933	0,704		0,293	100,00

Table S17 (continued)

		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	∑
Mol G	*k*	81	94	10	14	1		31	6	2	3	242
	d_{min}	2,388	2,503	3,303	1,862	3,363		2,494	3,407	3,404	3,650	1,86
	d_{max}	4,553	4,285	3,830	3,667	3,363		4,429	4,193	3,433	4,137	4,55
	S	127,009	74,571	3,617	24,652	0,477		57,806	3,199	0,071	0,864	292,26
	V	61,464	39,149	2,134	10,781	0,268		28,090	2,080	0,041	0,532	144,54
	Δ_S	43,457	25,515	1,237	8,435	0,163		19,778	1,095	0,024	0,296	100,00
Mol H	*k*	80	96	9	14	1		31	6	2	3	242
	d_{min}	2,388	2,503	3,293	1,862	3,367		2,483	3,334	3,404	3,657	1,86
	d_{max}	4,545	4,292	3,789	3,704	3,367		4,448	4,194	3,433	4,167	4,55
	S	127,461	74,705	3,556	24,728	0,610		57,508	3,151	0,071	0,902	292,69
	V	61,489	39,217	2,090	10,766	0,343		27,721	2,047	0,041	0,553	144,26
	Δ_S	43,548	25,523	1,215	8,449	0,208		19,648	1,077	0,024	0,308	100,00
Mol I	*k*	92	110	2	11	2		27	5	2		251
	d_{min}	2,208	2,356	3,303	1,794	3,363		2,467	3,605	3,595		1,79
	d_{max}	4,585	4,659	3,366	4,353	4,352		4,448	4,194	3,608		4,66
	S	153,450	79,566	0,054	20,461	1,432		44,678	4,267	0,148		304,05
	V	77,320	43,862	0,030	8,345	0,960		22,822	2,727	0,089		156,15
	Δ_S	50,468	26,168	0,018	6,729	0,471		14,694	1,403	0,049		100,00
Mol J	*k*	90	112	2	11	2		27	5	2		251
	d_{min}	2,208	2,356	3,293	1,794	3,367		2,483	3,580	3,595		1,79
	d_{max}	4,669	4,682	3,368	4,351	4,358		4,429	4,193	3,608		4,68
	S	154,605	78,761	0,082	20,352	1,619		44,247	4,649	0,148		304,46
	V	77,819	43,449	0,046	8,312	1,075		22,631	2,959	0,089		156,38
	Δ_S	50,780	25,869	0,027	6,685	0,532		14,533	1,527	0,048		100,00