Sublimation of pyridine derivatives: Fundamental aspects and application for two-component crystals screening

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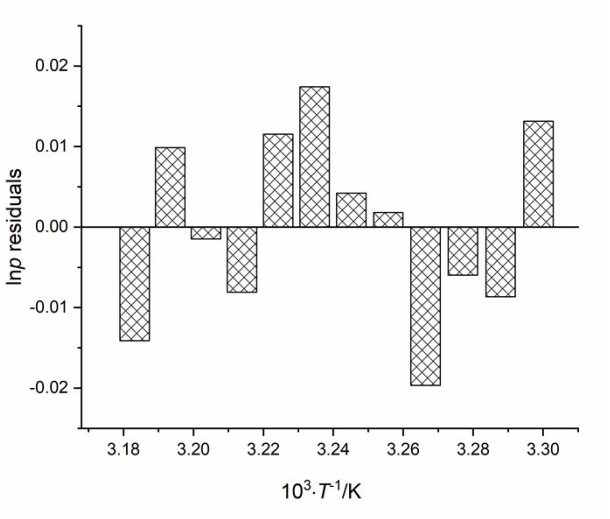

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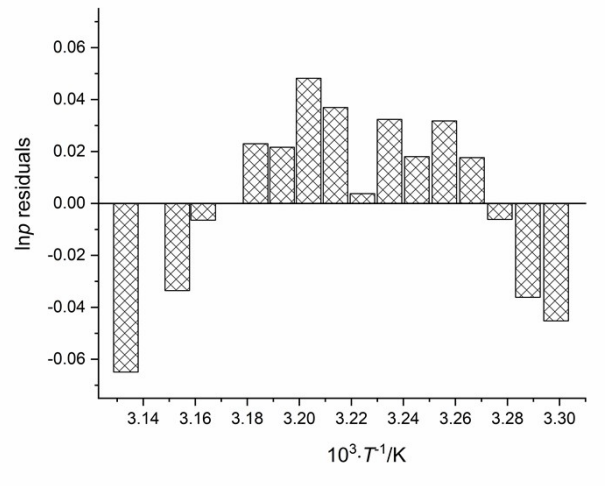

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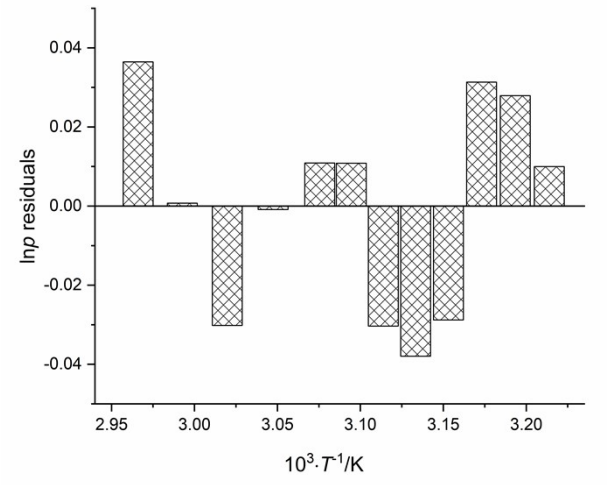

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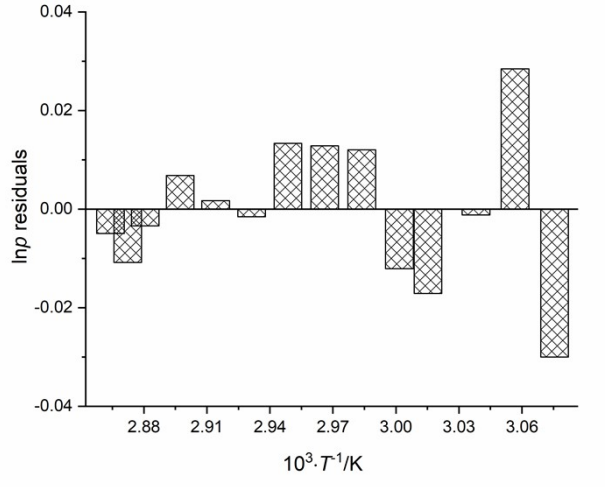

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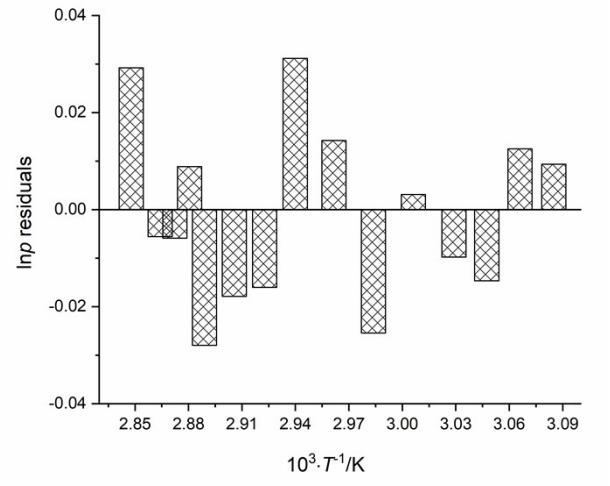
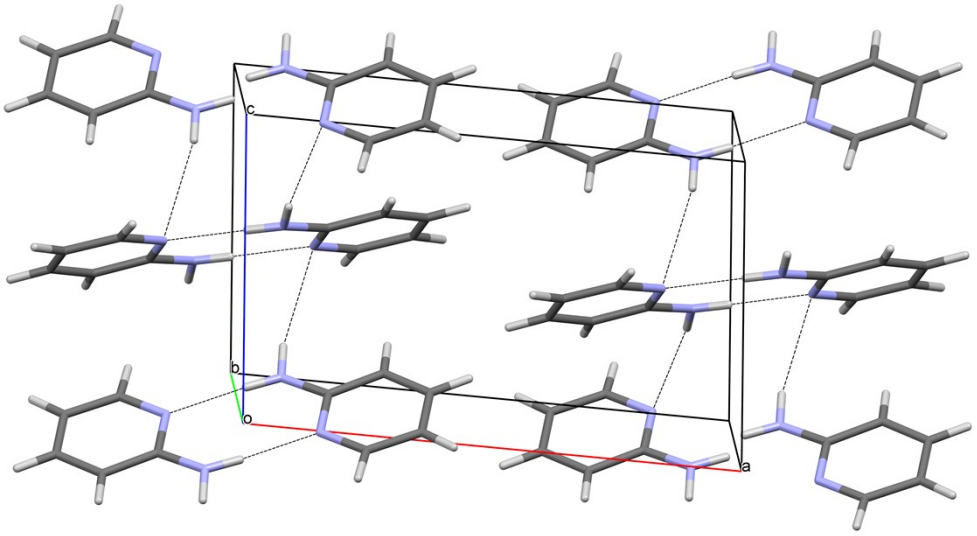
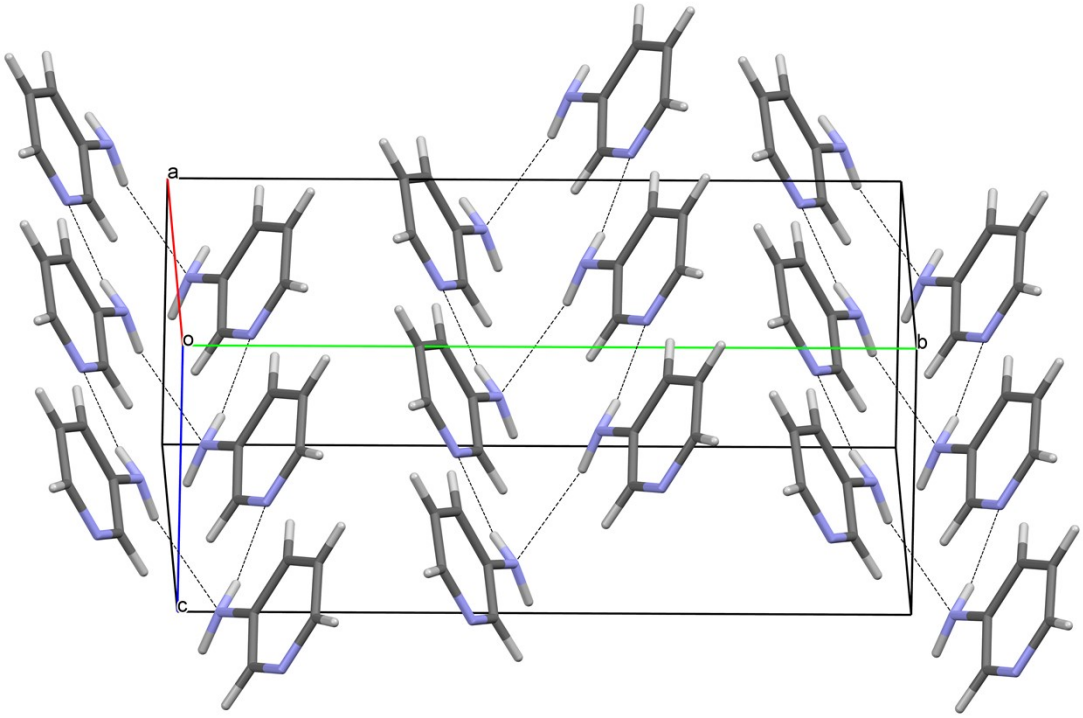


(e)

Figure S1. The diagrams of the residuals (ln*p* (exp) – ln*p* (regression) as a function of temperature for the compounds under study: 2AmPy (a), 3AmPy (b), 4AmPy (c), .3OHPy (d), ImPy (e).



(a)



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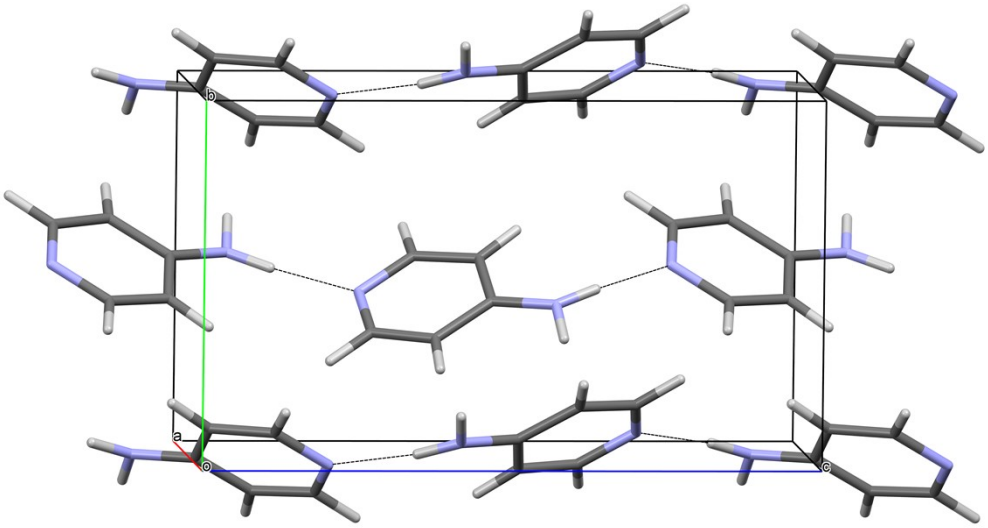

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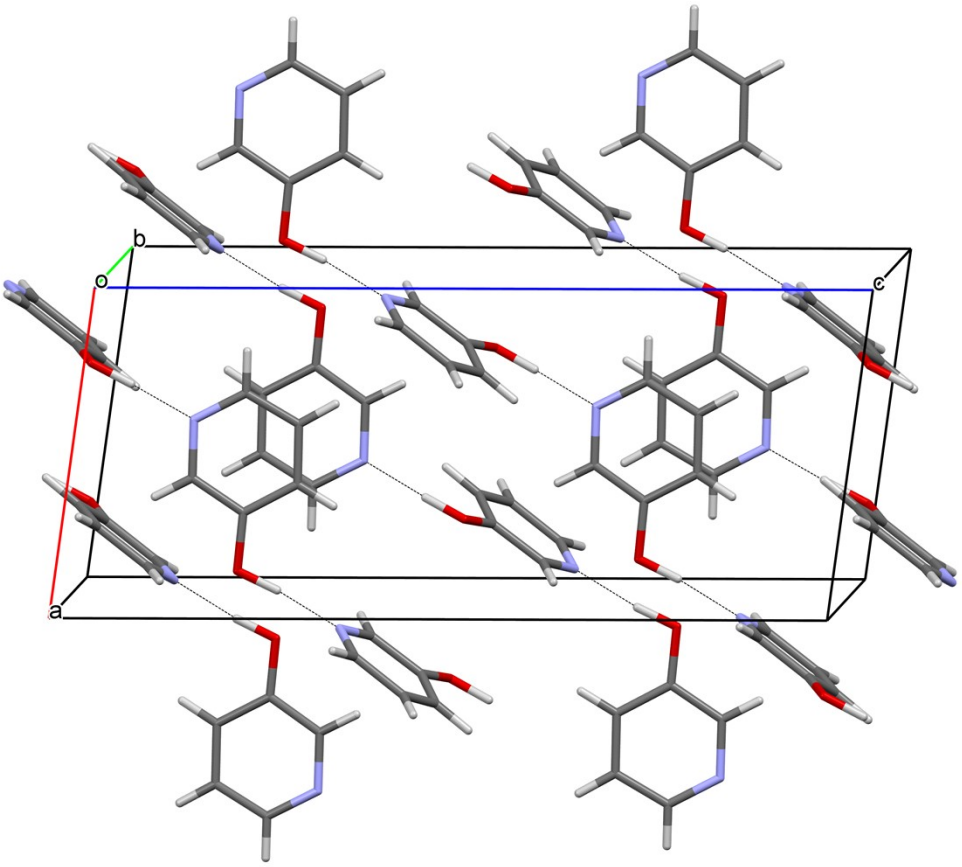

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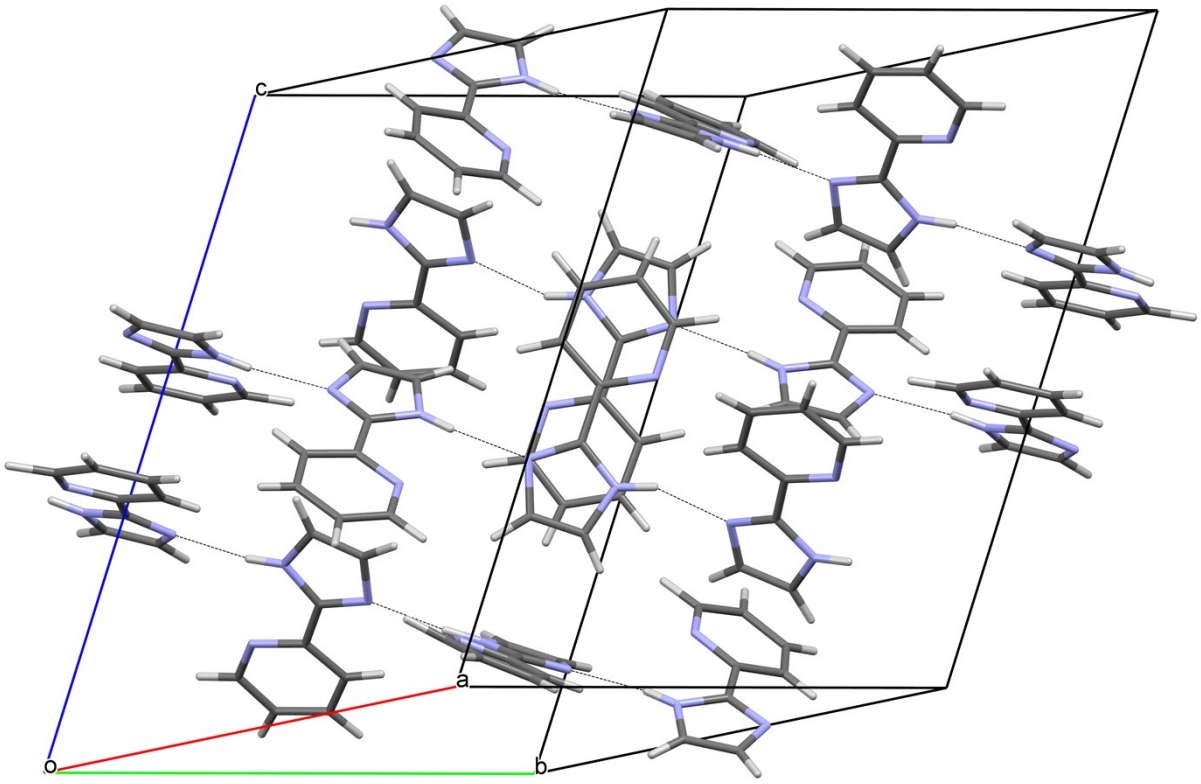

(e)

Figure S2. Molecular packing in crystals of studied pyridine derivatives: 2AmPy (a), 3AmPy (a), 4AmPy (c), 3OHPy (d), ImPy (e).

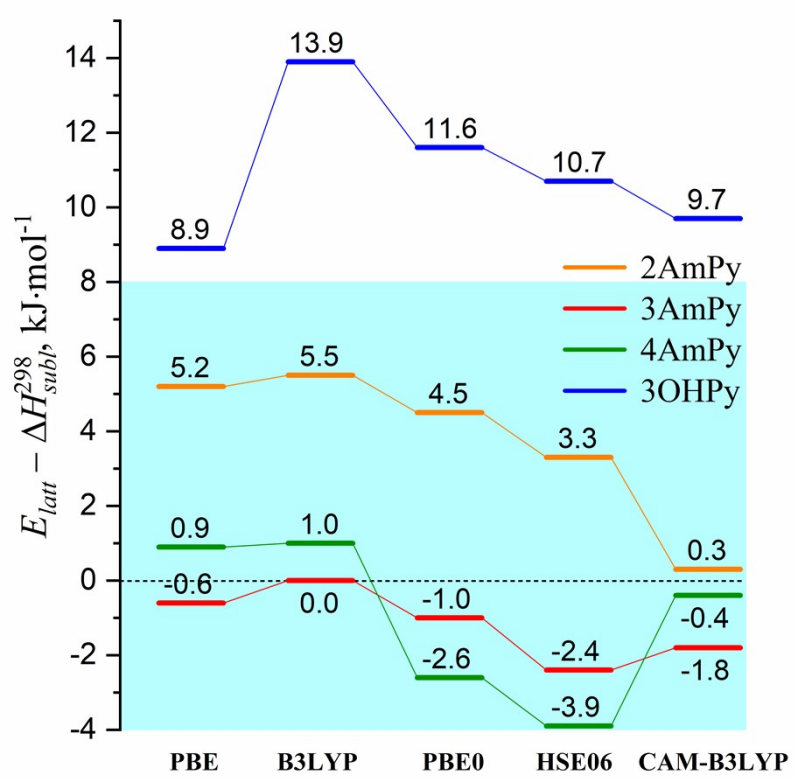

Figure S3. Difference between the experimental sublimation enthalpy and lattice energy estimated using eq. (15) based on periodic DFT-D3 computations using different functionals with lattice parameters optimised during structure relaxation. The tolerance range of ±8 kJ·mol^{-1} from the experimental value is given in cyan.

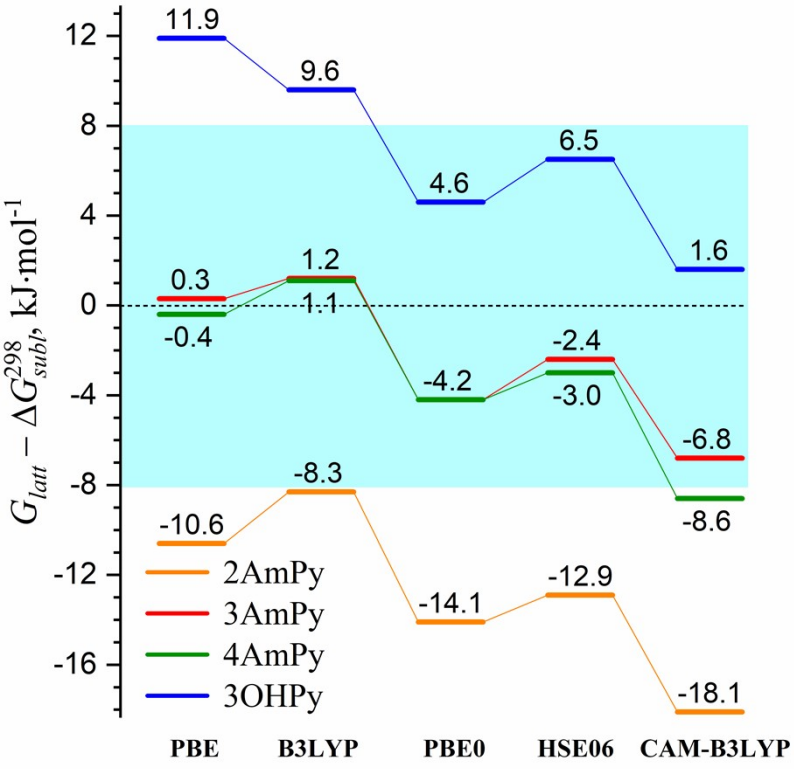

Figure S4. Difference between the experimental sublimation Gibbs energy and lattice Gibbs energy estimated using eq. (14) based on periodic DFT-D3 computations using different functionals with lattice parameters fixed during structure relaxation. The tolerance range of ±8 kJ·mol^{-1} from the experimental value is given in cyan.

Table S1. Compounds used in this study.

Compound	CASRN	Source	Mass fraction purity, %	
			Stated	Observed
2-Aminopyridine (2AmPy)	504-29-0	Aldrich	≥98	99.6
3-Aminopyridine (3AmPy)	462-08-08	Aldrich	≥99	99.2
4-Aminopyridine (4AmPy)	504-24-5	Aldrich	≥98	99.1
3-Hydroxypyridine (3OHPy)	109-00-2	Aldrich	≥98	99.7
2-(1H-Imidazol-2-yl)pyridine (ImPy)	18653-75-3	Aldrich	≥97	99.4

Table S2. Molecular volumes (V_{vdw}) of molecules extracted from crystals of studied compounds, unit cell volumes (V_{cell}), number of molecules in the unit cell (Z^*Z'), free volumes (V_{free}) and packing parameters (β). For 2AmPy, two structures with diffraction data collected at different temperatures (T) were used.

Compound	CSD ID	Space group	V_{vdw}, Å^3	V_{cell}, Å^3	Z^*Z'	V_{cell}, Å^3 per 1 mol.	V_{free}, Å^3 per 1 mol.	β V_{free}/V_{vdw}	T, K
2AmPy	AMPYRD	$P2_1/c$	86.73980	502.068	4	125.517	38.7772	0.309534	RT
	AMPYRD01	$P2_1/c$	86.91360	486.291	4	121.57275	34.65915	0.398777	150
3AmPy	AMIPYR	C c	86.63506	506.271	4	126.56775	39.93269	0.46093	RT
4AmPy	AMPYRE01	$P2_12_12_1$	87.67611	477.325	4	119.33125	31.65514	0.361046	RT
3OHPy	BIRYIK11	$P2_1/c$	84.64698	946.678	8	118.3348	33.68777	0.39798	RT
ImPy	EHUKIC	P-1	126.8329	2878.94	16	179.9338	53.10088	0.418668	RT

Table S3. Vapour pressures (p), sublimation enthalpies (H^T_{sub}), Gibbs energies (G^T_{sub}), and entropies (S^T_{sub}) measured using the transpiration technique.

T, K[a]	m, mg[b]	$V(N_2)$[c], dm^3	T_a, K[d]	Flow, dm^3·h^{-1}	p, Pa[e]	$u(p)$, Pa	G^T_{sub}, kJ·mol^{-1}	S^T_{sub}, J·K^{-1}·mol^{-1}
2AmPy: H^T_{sub} = (76.5 ± 0.9) kJ·mol^{-1}								
ln(p[Pa]) = (32.6 ± 0.4) – (9202 ± 350)/T, R^2=0.9989								
303.15	0.35	1.08	295.15	1.90	8.49	0.24	34.38	138.95
304.15	0.33	0.95	295.15	1.90	9.18	0.25	34.69	137.48
305.15	0.43	1.11	294.65	1.90	10.16	0.28	35.06	135.81
306.15	0.50	1.17	295.85	1.90	11.06	0.30	35.39	134.29
307.15	0.45	0.95	295.05	1.90	12.45	0.34	35.81	132.49
308.15	0.50	0.95	295.50	1.90	13.75	0.37	36.18	130.85
309.15	0.69	1.17	295.75	1.90	15.34	0.41	36.58	129.14
310.15	0.61	0.95	295.75	1.90	16.78	0.44	36.93	127.60
311.15	0.66	0.95	295.55	1.90	18.10	0.48	37.24	126.18
312.15	0.87	1.14	295.80	1.90	20.02	0.53	37.62	124.55
313.15	0.81	0.95	295.65	1.90	22.24	0.58	38.02	122.89
314.15	0.87	0.95	296.15	1.90	23.83	0.62	38.32	121.54
3AmPy: H^T_{sub} = (80.3 ± 1.5) kJ·mol^{-1}								
ln(p[Pa]) = (32.2 ± 0.6) – (9660 ± 177)/T, R^2=0.9952								
303.15	0.10	2.41	295.40	1.90	1.13	$0.91\cdot10^{-2}$	29.29	168.27
304.15	0.10	2.09	295.80	1.90	1.26	$0.98\cdot10^{-2}$	29.67	166.46
305.15	0.22	4.02	295.70	1.90	1.45	$1.25\cdot10^{-2}$	30.11	164.47
306.15	0.13	2.03	297.10	1.90	1.64	$1.35\cdot10^{-2}$	30.53	162.56
307.15	0.13	1.90	295.45	1.90	1.85	$1.83\cdot10^{-2}$	30.93	160.73
308.15	0.13	1.74	296.40	1.90	2.02	$2.09\cdot10^{-2}$	31.26	159.14
309.15	0.18	2.12	295.95	1.90	2.26	$2.76\cdot10^{-2}$	31.66	157.34
310.15	0.31	3.36	296.05	1.90	2.43	$3.20\cdot10^{-2}$	31.95	155.90
311.15	0.22	2.09	295.65	1.90	2.78	$4.23\cdot10^{-2}$	32.40	153.96
312.15	0.28	2.31	294.65	1.90	3.11	$6.06\cdot10^{-2}$	32.79	152.21
313.15	0.45	3.48	294.55	1.90	3.34	$8.34\cdot10^{-2}$	33.08	150.79
314.15	0.22	1.58	296.15	1.90	3.69	$0.91\cdot10^{-2}$	33.45	149.14
316.15	0.34	2.03	295.55	1.90	4.36	$0.98\cdot10^{-2}$	34.10	146.15
317.15	0.29	1.65	295.65	1.90	4.67	$1.25\cdot10^{-2}$	34.39	144.17
4AmPy: H^T_{sub} = (86.7 ± 0.9) kJ·mol^{-1}								
ln(p[Pa]) = (32.1 ± 0.3) – (10423 ± 103)/T, R^2=0.9990								

311.15	0.01	1.49	297.25	1.90	$2.26 \cdot 10^{-1}$	$0.60 \cdot 10^{-2}$	33.59	170.68
313.15	0.02	1.49	297.40	1.90	$2.85 \cdot 10^{-1}$	$0.91 \cdot 10^{-2}$	33.21	170.83
315.15	0.03	2.12	297.00	1.90	$3.54 \cdot 10^{-1}$	$0.98 \cdot 10^{-2}$	32.86	170.85
317.15	0.05	3.48	297.85	1.90	$4.10 \cdot 10^{-1}$	$1.25 \cdot 10^{-2}$	32.67	170.35
319.15	0.04	2.12	297.25	1.90	$4.99 \cdot 10^{-1}$	$1.35 \cdot 10^{-2}$	32.36	170.28
321.15	0.05	2.12	297.25	1.90	$6.17 \cdot 10^{-1}$	$1.83 \cdot 10^{-2}$	32.00	170.34
323.15	0.05	1.81	295.65	1.90	$7.86 \cdot 10^{-1}$	$2.09 \cdot 10^{-2}$	31.55	170.68
325.15	0.07	1.81	295.65	1.90	$9.58 \cdot 10^{-1}$	$2.76 \cdot 10^{-2}$	31.20	170.68
328.15	0.10	1.96	296.10	1.90	1.27	$3.20 \cdot 10^{-2}$	32.03	160.62
331.15	0.11	1.71	295.30	1.90	1.64	$4.23 \cdot 10^{-2}$	33.03	162.07
334.15	0.1	1.87	295.65	1.90	2.25	$6.06 \cdot 10^{-2}$	34.20	157.12
337.15	0.21	1.81	296.65	1.90	3.08	$8.34 \cdot 10^{-2}$	35.38	152.20
3OHPy: H^{T}_{sub} = (102.0 ± 0.4) kJ·mol^{-1} ln(p[Pa]) = (36.5 ± 0.2) – (12266 ± 52)/T, R^2=0.9998								
323.15	0.05	8.04	294.55	2.65	$1.48 \cdot 10^{-1}$	$0.71 \cdot 10^{-2}$	36.03	204.15
325.15	0.06	9.10	294.50	2.65	$1.80 \cdot 10^{-1}$	$0.85 \cdot 10^{-2}$	35.72	203.85
327.15	0.06	6.94	294.55	2.65	$2.48 \cdot 10^{-1}$	$0.92 \cdot 10^{-2}$	35.15	204.33
329.15	0.10	8.48	294.75	2.65	$2.94 \cdot 10^{-1}$	$0.98 \cdot 10^{-2}$	34.82	204.09
331.65	0.12	8.39	295.10	2.65	$3.83 \cdot 10^{-1}$	$1.46 \cdot 10^{-2}$	34.36	203.95
333.15	0.18	10.28	294.95	2.65	$4.54 \cdot 10^{-1}$	$1.64 \cdot 10^{-2}$	34.04	204.00
335.15	0.07	3.09	295.65	2.65	$5.80 \cdot 10^{-1}$	$1.95 \cdot 10^{-2}$	33.56	204.20
337.15	0.09	3.36	295.65	2.65	$7.21 \cdot 10^{-1}$	$2.30 \cdot 10^{-2}$	33.15	204.20
339.15	0.09	2.56	296.65	2.65	$8.94 \cdot 10^{-1}$	$2.74 \cdot 10^{-2}$	32.74	204.21
341.15	0.13	3.11	295.65	2.65	1.09	$3.22 \cdot 10^{-2}$	32.86	202.67
343.15	0.26	5.04	296.65	2.65	1.35	$3.87 \cdot 10^{-2}$	33.66	199.16
345.15	0.18	2.83	296.15	2.65	1.66	$4.66 \cdot 10^{-2}$	34.46	195.67
347.15	0.18	2.25	297.65	2.65	2.02	$5.56 \cdot 10^{-2}$	35.22	192.35
348.15	0.40	4.64	297.15	2.65	2.22	$6.06 \cdot 10^{-2}$	35.60	190.73
349.15	0.28	2.96	297.15	2.65	2.47	$6.68 \cdot 10^{-2}$	36.01	189.00
ImPy: H^{T}_{sub} = (107.2 ± 0.5) kJ·mol^{-1} ln(p[Pa]) = (38.8 ± 0.2) – (12893 ± 64)/T, R^2=0.9997								
324.15	0.07	10.60	294.95	2.65	$3.67 \cdot 10^{-1}$	$8.44 \cdot 10^{-3}$	33.70	226.76
326.15	0.04	4.55	294.65	2.65	$4.69 \cdot 10^{-1}$	$1.08 \cdot 10^{-2}$	33.23	226.78
328.15	0.04	3.80	294.40	2.65	$5.81 \cdot 10^{-1}$	$1.10 \cdot 10^{-2}$	32.86	226.56
330.15	0.07	5.04	294.25	2.65	$7.41 \cdot 10^{-1}$	$1.41 \cdot 10^{-2}$	32.39	226.60
332.65	0.09	4.99	295.55	2.65	1.01	$1.92 \cdot 10^{-2}$	31.82	226.59

335.15	0.11	5.04	294.80	2.65	1.31	$3.80 \cdot 10^{-2}$	32.79	222.02
337.65	0.08	2.65	294.75	2.65	1.81	$5.25 \cdot 10^{-2}$	33.94	216.96
340.15	0.19	4.42	294.15	2.65	2.43	$5.59 \cdot 10^{-2}$	35.04	212.15
342.15	0.28	5.57	294.15	2.65	2.90	$6.67 \cdot 10^{-2}$	35.74	208.86
344.15	0.22	3.58	297.65	2.65	3.60	$8.28 \cdot 10^{-2}$	36.57	205.23
346.15	0.16	2.03	297.15	2.65	4.42	$1.02 \cdot 10^{-1}$	37.38	201.72
347.15	0.20	2.21	296.90	2.65	5.11	$1.02 \cdot 10^{-1}$	37.90	199.63
348.15	0.27	2.78	297.65	2.65	5.60	$1.12 \cdot 10^{-1}$	38.27	197.98
349.15	0.29	2.65	297.40	2.65	6.23	$1.79 \cdot 10^{-1}$	38.69	196.21
351.15	0.43	3.09	297.15	2.65	7.96	$2.63 \cdot 10^{-1}$	39.63	192.42

[a] Saturation temperature with $u(T)$=0.1 K; [b] Mass of transferred sample condensed at T=273 K; [c] Volume of nitrogen ($u(V)$=0.005 dm^3) used to transfer a sample of mass m with $u(m)$=0.0001 g; [d] T_a is the temperature of the soap bubble meter used for measurement of the gas flow; [e] Vapour pressure at temperature T calculated from the m and the residual vapour pressure at T=273 K calculated by an iteration;

Table S4. Metric and energetic parameters of selected hydrogen bonds in the studied crystals optimised using different functionals. The interaction energies are estimated from QTAIMC data according to eq. (15).

Crystal	Relaxed unit cell parameters				Fixed unit cell parameters			
H-bond	D(D···A), Å	D(H···A), Å	∠D–H···A, °	E_{int}, kJ·mol^{-1}	D(D···A), Å	D(H···A), Å	∠D–H···A, °	E_{int}, kJ·mol^{-1}
2AmPy N_{am}-H···N_{py} (in plane)								
PBE	2.971	1.963	177.5	23.0	3.046	2.015	177.4	18.9
B3LYP	3.010	1.993	176.1	21.0	3.117	2.100	177.0	15.9
PBE0	3.003	1.985	176.4	21.5	3.086	2.068	177.2	17.3
HSE06	3.000	1.981	176.6	21.6	3.080	2.062	177.3	17.5
CAM-B3LYP	3.045	2.030	176.0	19.4	3.132	2.117	177.0	15.5
Exp.					**3.071**	**2.171**	**174.6**	
2AmPy N_{am}-H···N_{py} (out of plane)								
PBE	3.122	2.191	151.0	13.3	3.317	2.367	154.7	8.4
B3LYP	3.129	2.220	149.1	12.9	3.332	2.394	154.1	8.2
PBE0	3.138	2.226	149.6	12.7	3.332	2.395	154.2	8.2
HSE06	3.145	2.229	150.2	12.6	3.336	2.399	154.2	8.1
CAM-B3LYP	3.173	2.271	148.1	11.6	3.355	2.428	152.6	7.7
Exp.					**3.320**	**2.509**	**152.6**	
3AmPy N_{am}-H···N_{py} (in plane)								
PBE	2.939	1.909	170.7	24.8	3.036	2.008	171.7	19.3
B3LYP	2.976	1.965	169.6	22.8	3.097	2.086	170.5	16.7
PBE0	2.982	1.971	169.3	22.5	3.097	2.086	170.4	16.8
HSE06	2.985	1.973	169.5	22.5	3.087	2.075	170.7	17.2
CAM-B3LYP	3.022	2.016	169.5	20.4	3.133	2.128	169.5	15.4
Exp.					**3.123**	**2.216**	**167.8**	
3AmPy N_{am}-H···N_{py} (out of plane)								
PBE	3.249	2.310	152.4	10.3	3.389	2.436	154.9	7.4
B3LYP	3.233	2.310	151.4	10.7	3.372	2.427	155.0	7.8
PBE0	3.223	2.294	152.3	11.1	3.364	2.419	155.2	8.0
HSE06	3.251	2.310	152.7	10.9	3.370	2.426	155.1	7.9
CAM-B3LYP	3.258	2.340	150.9	10.1	3.370	2.428	154.9	8.0
Exp.					**3.336**	**2.455**	**161.5**	
4AmPy N_{am}-H···N_{py}								
PBE	2.885	1.855	169.0	28.2	2.959	1.930	170.5	23.3
B3LYP	2.931	1.924	167.2	25.1	3.028	2.017	169.9	19.7
PBE0	2.923	1.914	167.9	25.8	3.006	1.994	170.1	20.9
HSE06	2.918	1.906	168.3	26.1	2.997	1.983	170.2	21.4
CAM-B3LYP	2.967	1.966	166.8	23.1	3.053	2.047	169.3	18.6
Exp.					**2.983**	**2.061**	**167.2**	
3OHPy O1-H···N_{py}								
PBE	2.564	1.480	178.9	59.7	2.606	1.541	177.1	52.7
B3LYP	2.612	1.582	178.8	52.2	2.669	1.649	177.9	44.3
PBE0	2.587	1.551	179.6	55.9	2.641	1.619	177.7	48.0
HSE06	2.584	1.545	179.6	56.3	2.636	1.611	177.6	48.5
CAM-B3LYP	2.628	1.610	178.8	50.1	2.683	1.673	178.2	42.9
Exp.					**2.660**	**1.645**	**178.0**	
3OHPy O1'-H···N_{py}								
PBE	2.577	1.505	175.0	56.9	2.611	1.551	176.1	51.6
B3LYP	2.628	1.605	175.4	49.3	2.675	1.658	177.3	43.5
PBE0	2.605	1.579	175.5	52.6	2.650	1.632	176.7	46.6
HSE06	2.602	1.573	175.5	53.0	2.646	1.625	176.6	47.0
CAM-B3LYP	2.645	1.633	176.0	47.3	2.691	1.683	177.5	41.9
Exp.					**2.669**	**1.671**	**174.2**	

Table S5. Experimental and calculated lattice parameters of studied pyridine derivatives after DFT-D3 optimisation using various functionals with pob-TZVP_rev2 basis set and D3(BJ,ABC) dispersion correction.

	Experiment	PBE	B3LYP	PBE0	HSE06	CAM-B3LYP
2AmPy						
a, Å	11.6923(11)	11.40108	11.33357	11.36300	11.37420	11.37580
b, Å	5.6638(5)	5.564180	5.542882	5.558577	5.563035	5.589152
c, Å	7.3786(6)	6.756848	6.696704	6.712705	6.753332	6.735131
β, °	95.611(3)	94.94098	93.96468	93.90913	94.33487	93.46222
V, Å^3	486.29(7)	427.0459	419.6844	423.0020	426.0952	427.4455
$(V_{calc}-V_{exp})/V_{exp}$		-0.12183	-0.13697	-0.13015	-0.12379	-0.12101
3AmPy						
a, Å	6.186(4)	6.106422	6.100415	6.092444	6.095841	6.120995
b, Å	15.298(6)	13.40003	13.26129	13.39804	13.47737	13.37835
c, Å	5.713(3)	5.559682	5.564347	5.543252	5.542358	5.603884
β, °	110.54(3)	109.9527	110.8129	110.3074	110.2332	111.0750
V, Å^3	506.271	427.6206	420.7778	424.3538	427.2397	428.2004
$(V_{calc}-V_{exp})/V_{exp}$		-0.15535	-0.16887	-0.1618	-0.1561	-0.15421
4AmPy						
a, Å	5.5138(4)	5.182291	5.222734	5.246575	5.231825	5.277404
b, Å	7.1866(5)	6.940303	6.816715	6.834400	6.894715	6.875070
c, Å	12.0459(4)	11.77596	11.66765	11.69457	11.72065	11.67469
V, Å^3	477.32(5)	423.5421	415.3903	419.3345	422.7864	423.5873
$(V_{calc}-V_{exp})/V_{exp}$		-0.11267	-0.12975	-0.12149	-0.11426	-0.11258
3OHPy						
a, Å	7.6672(11)	7.573161	7.514249	7.544383	7.563160	7.534602
b, Å	7.0148(8)	6.655495	6.568473	6.632293	6.646602	6.605560
c, Å	17.803(2)	16.72301	16.70496	16.68930	16.71203	16.78771
β, °	98.628(3)	96.45126	97.03770	96.61034	96.59578	96.81045
V, Å^3	946.678	837.5547	818.2970	829.5234	834.5420	829.6332
$(V_{calc}-V_{exp})/V_{exp}$		-0.11527	-0.13561	-0.12375	-0.11845	-0.12364

Table S6. Total electronic energies of crystals (E^{cryst}) and isolated molecules (E^{mol}), zero-point energies (ZPE), basis set superposition energy (BSSE) and thermal corrections (E_{therm}), pressure-volume term (pV), entropy corrections (TS), total enthalpies and free Gibbs energies of crystals and molecules (H^{cryst}, H^{mol}, G^{cryst}, G^{mol}), Cocrystal Formation Energies (E_{form}) and Cocrystal Formation Gibbs Energies (E_{form}) obtained from periodic DFT-D3 calculations with various functionals (fixed cell optimisation). The units are a.u. per unit cell and kJ·mol^{-1}.

Crystal	PBE	B3LYP	PBE0	HSE06	CAM-B3LYP
2AmPy crystal (Z = 4)					
E^{cryst}, a.u./cell	-1213.578002485210	-1214.390623339990	-1213.634187033930	-1213.604892425410	-1214.411114491930
ZPE, a.u./cell	0.418533068754	0.431609984371	0.433715574883	0.433314081684	0.436531434712
E_{therm}, a.u./cell	0.025757190966	0.025013316004	0.025175504939	0.025180962050	0.024860890144
pV, a.u./cell	0.000011301904	0.000011301904	0.000011301904	0.000011301904	0.000011301904
H^{cryst}, a.u./cell	-1213.133700923590	-1213.933988737710	-1213.175284652200	-1213.146386079770	-1213.949710865170
TS, a.u./cell	0.051112314466	0.049618790715	0.050418435337	0.050397195181	0.049546289361
G^{cryst}, a.u./cell	-1213.184813238050	-1213.983607528430	-1213.225703087540	-1213.196783274950	-1213.999257154520
2AmPy molecule					
E^{mol}, a.u./cell	-303.338613457892	-303.540168786878	-303.355752810676	-303.348010639876	-303.549187439891
ZPE, a.u./cell	0.102904756209	0.105667272174	0.106539412523	0.106457659630	0.106944902807
E_{therm}, a.u./cell	0.005768606758	0.005611467906	0.005584421418	0.005588833340	0.005556811515
pV, a.u./cell	0.000944185937	0.000944185937	0.000944185937	0.000944185937	0.000944185937
H^{mol}, a.u./cell	-303.228995908988	-303.427945860861	-303.242684790798	-303.235019960969	-303.435741539632
TS, a.u./cell	0.034790402804	0.034521660009	0.034471610795	0.034478205517	0.034424413181
G^{mol}, a.u./cell	-303.263786311792	-303.462467520870	-303.277156401593	-303.269498166486	-303.470165952813
BSSE, kJ·mol^{-1}	-62.92729696	-63.29989831	-58.11331409	-58.06869644	-63.13069135
E_{latt}, kJ·mol^{-1}	**79.266245**	**81.76376613**	**75.536363**	**76.72868928**	**71.82848172**
H_{latt}, kJ·mol^{-1}	**79.97688771**	**82.55010171**	**76.14523126**	**77.34555914**	**72.57136548**
G_{latt}, kJ·mol^{-1}	**22.18353056**	**24.48201712**	**18.73341762**	**19.90248954**	**14.71101435**
3AmPy crystal (Z = 2)					
E^{cryst}, a.u./cell	-606.768829759173	-607.172736881514	-606.794690346048	-606.780326380005	-607.182847299632
ZPE, a.u./cell	0.207901561437	0.214352080036	0.215648543211	0.215419773579	0.216880998764
E_{therm}, a.u./cell	0.012008616947	0.011678026898	0.011683896824	0.011701041887	0.011580289475
pV, a.u./cell	0.000005883132	0.000005883132	0.000005883132	0.000005883132	0.000005883132
H^{cryst}, a.u./cell	-606.548913697657	-606.946700891448	-606.567352022881	-606.553199681407	-606.954380128261
TS, a.u./cell	0.024479622690	0.023798271278	0.023872579403	0.024010151868	0.023584231747
G^{cryst}, a.u./cell	-606.573393320346	-606.970499162726	-606.591224602285	-606.577209833274	-606.977964360008
3AmPy molecule					
E^{mol}, a.u./cell	-303.329633092221	-303.530887059948	-303.345810276472	-303.338064231529	-303.539209944549
ZPE, a.u./cell	0.102578364964	0.105380721504	0.106218175025	0.106133246814	0.106674791175
E_{therm}, a.u./cell	0.005857244376	0.005701073851	0.005685017710	0.005688647813	0.005647433776
pV, a.u./cell	0.000944185937	0.000944185937	0.000944185937	0.000944185937	0.000944185937
H^{mol}, a.u./cell	-303.220253296944	-303.418861078656	-303.232962897800	-303.225298150965	-303.425943533661
TS, a.u./cell	0.035019493347	0.034770784168	0.034737204644	0.034741987230	0.034682167789
G^{mol}, a.u./cell	-303.255272790291	-303.453631862824	-303.267700102444	-303.260040138195	-303.460625701450
BSSE, kJ·mol^{-1}	-53.15330492	-52.66767682	-48.38148201	-48.33004665	-52.17794036
E_{latt}, kJ·mol^{-1}	**87.07300025**	**88.28507974**	**82.70658231**	**84.31630056**	**80.27327592**
H_{latt}, kJ·mol^{-1}	**89.15812055**	**90.39415642**	**84.76579785**	**86.36253975**	**82.36982539**
G_{latt}, kJ·mol^{-1}	**29.35006546**	**30.34464321**	**24.90199567**	**26.66677915**	**22.27199408**
4AmPy crystal (Z = 4)					
E^{cryst}, a.u./cell	-1213.584282460410	-1214.396135278420	-1213.639171699820	-1213.609917445220	-1214.415924107290
ZPE, a.u./cell	0.418562725763	0.431620387279	0.433845266167	0.433475240619	0.436836089635
E_{therm}, a.u./cell	0.025655164712	0.025033241410	0.025105324822	0.025100038453	0.024786958416
pV, a.u./cell	0.000011093520	0.000011093520	0.000011093520	0.000011093520	0.000011093520
H^{cryst}, a.u./cell	-1213.140053476420	-1213.939470556210	-1213.180210015310	-1213.151331072630	-1213.954289965720
TS, a.u./cell	0.049917635544	0.048715253149	0.049131797920	0.049135500225	0.048204449278
G^{cryst}, a.u./cell	-1213.189971111960	-1213.988185809360	-1213.229341813230	-1213.200466572850	-1214.002494415000

4AmPy molecule					
E^{mol}, a.u./cell	-303.333763558203	-303.535379763779	-303.350530663369	-303.342806873949	-303.544021145360
ZPE, a.u./cell	0.102862854104	0.105669434851	0.106516333099	0.106434752565	0.106943541172
E_{therm}, a.u./cell	0.005822618599	0.005657008795	0.005642823881	0.005647559681	0.005607547214
pV, a.u./cell	0.000944185937	0.000944185937	0.000944185937	0.000944185937	0.000944185937
H^{mol}, a.u./cell	-303.224133899563	-303.423109134196	-303.237427320452	-303.229780375766	-303.430525871037
TS, a.u./cell	0.034878722303	0.034600538904	0.034572901059	0.034580581247	0.034512950049
G^{mol}, a.u./cell	-303.259012621867	-303.457709673100	-303.272000221511	-303.264360957013	-303.465038821086
BSSE, kJ·mol^{-1}	-65.84712633	-66.61617831	-61.3671133	-61.26226892	-66.44682054
E_{latt}, kJ·mol^{-1}	**93.07236589**	**94.63781476**	**89.11940046**	**90.32997843**	**85.02982726**
H_{latt}, kJ·mol^{-1}	**93.99192095**	**95.53077619**	**89.92780565**	**91.1542873**	**85.95458131**
G_{latt}, kJ·mol^{-1}	**35.18252357**	**36.66253559**	**31.40553778**	**32.6142852**	**26.98102635**
3OHPy crystal (Z = 4)					
E^{cryst}, a.u./cell	-2586.009038751420	-2587.679572094030	-2586.061797542000	-2586.009760138440	-2587.753946168480
ZPE, a.u./cell	0.731484818687	0.758326425219	0.769097769561	0.761795154989	0.768834442609
E_{therm}, a.u./cell	0.051211916071	0.050521618264	0.050408720283	0.050348558830	0.050094591754
pV, a.u./cell	0.000022001793	0.000022001793	0.000022001793	0.000022001793	0.000022001793
H^{cryst}, a.u./cell	-2585.226320014870	-2586.870702048750	-2585.242269050360	-2585.197594422830	-2586.934995132320
TS, a.u./cell	0.107770671208	0.108603632771	0.108296500040	0.107448939098	0.107170437556
G^{cryst}, a.u./cell	-2585.334090686070	-2586.979305681530	-2585.356930520710	-2585.305043361920	-2587.042165569880
3OHPy molecule 1					
E^{mol}, a.u./cell	-323.189177005518	-323.398219359612	-323.199961555348	-323.192766732709	-323.410601525484
ZPE, a.u./cell	0.090295110639	0.092797041466	0.093623987831	0.093550273891	0.094031170653
E_{therm}, a.u./cell	0.005600642462	0.005470761547	0.005461481717	0.005461855949	0.005414362092
pV, a.u./cell	0.000944185937	0.000944185937	0.000944185937	0.000944185937	0.000944185937
H^{mol}, a.u./cell	-323.092337066480	-323.299007370662	-323.099931899863	-323.092810416932	-323.310211806802
TS, a.u./cell	0.034592690968	0.034383879925	0.034372760249	0.034371905743	0.034293784429
G^{mol}, a.u./cell	-323.126929757448	-323.333391250587	-323.134304660112	-323.127182322675	-323.344505591230
BSSE, kJ/mol	-53.54224407	-54.41543336	-49.10072684	-48.89027834	-53.93182763
3OHPy molecule 2					
E^{mol}, a.u./cell	-323.189173507302	-323.398217529504	-323.199959929466	-323.192765073390	-323.410599884735
ZPE, a.u./cell	0.090287820921	0.092830354790	0.093685442272	0.093608314755	0.094085502379
E_{therm}, a.u./cell	0.005587814621	0.005455774843	0.005425821534	0.005427730839	0.005394939683
pV, a.u./cell	0.000944185937	0.000944185937	0.000944185937	0.000944185937	0.000944185937
H^{mol}, a.u./cell	-323.092353685823	-323.298987213934	-323.099904479723	-323.092784841859	-323.310175256736
TS, a.u./cell	0.034560266141	0.034348066035	0.034289525074	0.034291875902	0.034246255091
G^{mol}, a.u./cell	-323.126913951964	-323.333335279968	-323.134194004797	-323.127076717760	-323.344421511827
BSSE, kJ·mol^{-1}	-51.41506384	-51.11993842	-47.0119693	-46.68198903	-50.57080496
E_{latt}, kJ·mol^{-1}	**107.179185**	**104.1084653**	**97.08508367**	**101.3659331**	**96.34304949**
H_{latt}, kJ·mol^{-1}	**107.5314608**	**104.3434518**	**97.30561859**	**101.60921**	**96.56428103**
G_{latt}, kJ·mol^{-1}	**52.11990355**	**49.75794448**	**44.79966483**	**46.73422932**	**41.76034213**

Table S7. Total electronic energies of crystals (E^{cryst}) and isolated molecules (E^{mol}), zero-point energies (ZPE), basis set superposition energy (BSSE) and thermal corrections (E_{therm}), pressure-volume term (pV), entropy corrections (TS), total enthalpies and free Gibbs energies of crystals and molecules (H^{cryst}, H^{mol}, G^{cryst}, G^{mol}), Cocrystal Formation Energies (E_{form}) and Cocrystal Formation Gibbs Energies (E_{form}) obtained from periodic DFT-D3 calculations with various functionals (relaxed cell optimisation). The units are a.u. per unit cell and kJ·mol^{-1}.

Crystal	PBE	B3LYP	PBE0	HSE06	CAM-B3LYP
2AmPy crystal (Z = 4)					
E^{cryst}, a.u./cell	-1213.591960598340	-1214.411288397490	-1213.650088949900	-1213.618749370070	-1214.427015350600
ZPE, a.u./cell	0.422590692207	0.437158134398	0.438160055566	0.437445854116	0.441454685099
E_{therm}, a.u./cell	0.023954944907	0.022958792170	0.023251830744	0.023380992006	0.022998332773
pV, a.u./cell	0.000009924993	0.000009753904	0.000009831009	0.000009902897	0.000009934280
H^{cryst}, a.u./cell	-1213.145405036230	-1213.951161717020	-1213.188667232580	-1213.157912621050	-1213.962552398450
TS, a.u./cell	0.044098590593	0.041884683356	0.042844384157	0.043280344560	0.042386212463
G^{cryst}, a.u./cell	-1213.189503626830	-1213.993046400380	-1213.231511616730	-1213.201192965610	-1214.004938610920
2AmPy molecule					
E^{mol}, a.u./cell	-303.338615099433	-303.540171373807	-303.355754016091	-303.348011956610	-303.549188896905
ZPE, a.u./cell	0.102936469999	0.105720703607	0.106564271276	0.106482621000	0.106993320979
E_{therm}, a.u./cell	0.005763943775	0.005596599709	0.005581813306	0.005586372091	0.005542053934
pV, a.u./cell	0.000944185937	0.000944185937	0.000944185937	0.000944185937	0.000944185937
H^{mol}, a.u./cell	-303.228970499722	-303.427909884554	-303.242663745572	-303.234998777582	-303.435709336055
TS, a.u./cell	0.034778906906	0.034492516726	0.034464519096	0.034471808524	0.034394632663
G^{mol}, a.u./cell	-303.263749406628	-303.462402401279	-303.277128264668	-303.269470586105	-303.470103968719
BSSE, kJ·mol^{-1}	-80.13148422	-82.67393986	-75.84169486	-74.99659144	-80.52359422
E_{latt}, kJ·mol^{-1}	**68.63944634**	**72.44557696**	**65.39045814**	**66.2462332**	**61.76430301**
H_{latt}, kJ·mol^{-1}	**70.52169942**	**74.54243025**	**67.25609592**	**68.03901466**	**63.69187450**
G_{latt}, kJ·mol^{-1}	**8.154891741**	**11.47438663**	**4.89148368**	**5.941417542**	**1.210016656**
3AmPy crystal (Z = 2)					
E^{cryst}, a.u./cell	-606.780063647358	-607.188409190144	-606.806691821298	-606.791193695554	-607.195262329967
ZPE, a.u./cell	0.210174157014	0.217529400486	0.218037505465	0.217644786356	0.219671701736
E_{therm}, a.u./cell	0.011005758608	0.010520125020	0.010657479452	0.010723967249	0.010542126701
pV, a.u./cell	0.000004969175	0.000004889657	0.000004931213	0.000004964749	0.000004975912
H^{cryst}, a.u./cell	-606.558878762561	-606.960354774981	-606.577991905168	-606.562819977200	-606.965043525618
TS, a.u./cell	0.019945256257	0.018870980288	0.019319491072	0.019539023358	0.019092011443
G^{cryst}, a.u./cell	-606.578824018817	-606.979225755269	-606.597311396240	-606.582359000559	-606.984135537062
3AmPy molecule					
E^{mol}, a.u./cell	-303.329632632479	-303.530884871957	-303.345810868558	-303.338064653216	-303.539206490788
ZPE, a.u./cell	0.102557779017	0.105334284907	0.106207190656	0.106120338961	0.106611875531
E_{therm}, a.u./cell	0.005859863434	0.005714769286	0.005686877525	0.005690172359	0.005663228932
pV, a.u./cell	0.000944185937	0.000944185937	0.000944185937	0.000944185937	0.000944185937
H^{mol}, a.u./cell	-303.220270804091	-303.418891631827	-303.232972614440	-303.225309955959	-303.425987200388
TS, a.u./cell	0.035022177567	0.034795507466	0.034738550357	0.034742503159	0.034711102148
G^{mol}, a.u./cell	-303.255292981657	-303.453687139293	-303.267711164797	-303.260052459118	-303.460698302535
BSSE, kJ·mol^{-1}	-76.50732129	-78.66923142	-71.66372684	-70.87160551	-76.0891615
E_{latt}, kJ·mol^{-1}	**75.4300794**	**78.57014615**	**72.01276994**	**73.08492796**	**68.84027335**
H_{latt}, kJ·mol^{-1}	**78.83977812**	**82.23652007**	**75.42554745**	**76.41903019**	**72.34233214**
G_{latt}, kJ·mol^{-1}	**13.07218607**	**15.65379459**	**9.581145397**	**10.85244106**	**6.271371474**
4AmPy crystal (Z = 4)					
E^{cryst}, a.u./cell	-1213.596380088170	-1214.414254285930	-1213.652740257300	-1213.621725264390	-1214.428968114280
ZPE, a.u./cell	0.421057199181	0.436067447001	0.437190974860	0.436396487606	0.440380470215
E_{therm}, a.u./cell	0.024381782580	0.023391273699	0.023627418627	0.023768277036	0.023460076749
pV, a.u./cell	0.000009843560	0.000009654104	0.000009745771	0.000009825997	0.000009844612
H^{cryst}, a.u./cell	-1213.150931262850	-1213.954785911130	-1213.191912118040	-1213.161550673750	-1213.965117722700
TS, a.u./cell	0.044896010982	0.042555150154	0.043443541584	0.043959740848	0.043096143678
G^{cryst}, a.u./cell	-1213.195827273830	-1213.997341061280	-1213.235355659620	-1213.205510414600	-1214.008213866380

4AmPy molecule					
E^{mol}, a.u./cell	-303.333763938616	-303.535380113211	-303.350531161577	-303.342807252941	-303.544021775543
ZPE, a.u./cell	0.102842445841	0.105660653169	0.106490778519	0.106408939853	0.106939671843
E_{therm}, a.u./cell	0.005825370907	0.005660227113	0.005647977923	0.005652209733	0.005607276078
pV, a.u./cell	0.000944185937	0.000944185937	0.000944185937	0.000944185937	0.000944185937
H^{mol}, a.u./cell	-303.224151935931	-303.423115046992	-303.237448219198	-303.229801917418	-303.430530641685
TS, a.u./cell	0.034885995813	0.034609142122	0.034584613407	0.034591244977	0.034513336803
G^{mol}, a.u./cell	-303.259037931745	-303.457724189113	-303.272032832605	-303.264393162395	-303.465043978489
BSSE, kJ·mol^{-1}	-80.32927823	-83.40901714	-76.29994118	-75.41664085	-80.91519639
E_{latt}, kJ·mol^{-1}	**84.83890375**	**86.79492692**	**80.82819336**	**81.93976399**	**76.78495522**
H_{latt}, kJ·mol^{-1}	**86.60232164**	**88.77502940**	**82.62107579**	**83.65124845**	**78.58074911**
G_{latt}, kJ·mol^{-1}	**24.47775883**	**25.84086344**	**20.33442790**	**21.68600966**	**16.25321463**
3OHPy crystal (Z = 4)					
E^{cryst}, a.u./cell	-2586.036214989090	-2587.719905180010	-2586.092686861790	-2586.037539360290	-2587.787611872600
ZPE, a.u./cell	0.736942534485	0.767167026879	0.769097769561	0.767636230107	0.776914732328
E_{therm}, a.u./cell	0.048373883375	0.046872040352	0.047263699058	0.047409576362	0.046794508378
pV, a.u./cell	0.000019465647	0.000019018078	0.000019278990	0.000019395629	0.000019281542
H^{cryst}, a.u./cell	-2585.250879105580	-2586.905847094700	-2585.276306114180	-2585.222474158190	-2586.963883350350
TS, a.u./cell	0.094051959716	0.090593538257	0.092475781082	0.093018729223	0.091244415253
G^{cryst}, a.u./cell	-2585.344931065300	-2586.996440632960	-2585.368781895260	-2585.315492887420	-2587.055127765600
3OHPy molecule 1					
E^{mol}, a.u./cell	-323.189176457691	-323.398218242404	-323.199961354246	-323.192766598483	-323.410600237620
ZPE, a.u./cell	0.090263437755	0.092736746023	0.093593774885	0.093521403962	0.093918622017
E_{therm}, a.u./cell	0.005613233803	0.005513829886	0.005477507390	0.005476549141	0.005490988845
pV, a.u./cell	0.000944185937	0.000944185937	0.000944185937	0.000944185937	0.000944185937
H^{mol}, a.u./cell	-323.092355600196	-323.299023480558	-323.099945886034	-323.092824459443	-323.310246440821
TS, a.u./cell	0.034612854043	0.034475510545	0.034402214697	0.034398256535	0.034475700391
G^{mol}, a.u./cell	-323.126968454240	-323.333498991103	-323.134348100731	-323.127222715977	-323.344722141212
BSSE, kJ·mol^{-1}	-72.18422820	-75.43122672	-67.92086036	-67.08279341	-73.66351616
3OHPy molecule 2					
E^{mol}, a.u./cell	-323.189173468971	-323.398217277953	-323.199960162138	-323.192765153924	-323.410600541187
ZPE, a.u./cell	0.090286575009	0.092823460517	0.093687658935	0.093609779635	0.094072168380
E_{therm}, a.u./cell	0.005588559727	0.005455226992	0.005424875427	0.005426725771	0.005395395555
pV, a.u./cell	0.000944185937	0.000944185937	0.000944185937	0.000944185937	0.000944185937
H^{mol}, a.u./cell	-323.092354148298	-323.298994404507	-323.099903441839	-323.092784462581	-323.310188791315
TS, a.u./cell	0.034562048627	0.034346441763	0.034287714445	0.034289909944	0.034246766101
G^{mol}, a.u./cell	-323.126916196925	-323.333340846270	-323.134191156285	-323.127074372525	-323.344435557416
BSSE, kJ·mol^{-1}	-65.42830355	-67.91544185	-61.43818462	-60.71153007	-66.50657697
E_{latt}, kJ·mol^{-1}	**97.93687585**	**95.45185013**	**90.56260433**	**92.41882509**	**90.32017847**
H_{latt}, kJ·mol^{-1}	**99.23889825**	**96.94138049**	**91.8359852**	**93.64546367**	**91.72653909**
G_{latt}, kJ·mol^{-1}	**39.29622230**	**36.32702944**	**32.01267612**	**34.00265732**	**31.45639773**

Table S8. Lattice energies E_{latt} of studied compounds estimated using parametrised force field schemes PIXEL and CE-B3LYP. The numbers in brackets display the discrepancies between calculated E_{latt} and experimental sublimation enthalpy at 298.15 K. All units are kJ·mol^{-1}.

Method \ Crystal	2AmPy	3AmPy	4AmPy	3OHPy
PIXEL	91.3 (+14.6)	93.6 (+13.1)	104.4 (+17.3)	102.8 (+0.2)
CE-B3LYP	90.2 (+13.5)	79.7 (-0.8)	101.1 (+14.0)	121.6 (+21.0)

Table S9. Contributions into the crystal lattice energy from different kinds of non-covalent interactions in crystals of pyridine derivatives estimated by QTAIMC depending on the functional used for optimisation and wave function calculation and given in kJ·mol^{-1} and % of total lattice energy value.

Method\Crystal	2AmPy		3AmPy		4AmPy		3OHPy	
PBE	fix.cell	opt.cell	fix.cell	opt.cell	fix.cell	opt.cell	fix.cell	opt.cell
E_{latt}(0K)	**53.9**	**81.9**	**50.5**	**79.9**	**58.3**	**88.0**	**84.0**	**110.8**
ΣE_{int}(N-H···N)	27.3 (50.7%)	36.3 (44.4%)	19.3 (38.3%)	24.8 (31.1%)	23.3 (40.0%)	28.2 (32.0%)	52.1 (62.0%)	58.3 (52.6%)
ΣE_{int}(N-H···C)	–	–	–	–	6.7 (11.5%)	10.3 (11.7%)	–	–
ΣE_{int}(C-H···X)	3.0 (5.6%)	5.3 (6.4%)	12.8 (25.4%)	15.4 (19.2%)	16.1 (27.7%)	25.6 (29.1%)	15.2 (18.1%)	29.8 (26.9%)
ΣE_{int}(C-H···π)	13.9 (25.7%)	24.9 (30.5%)	13.1 (25.9%)	32.8 (41%)	9.4 (16.1%)	13.9 (15.8%)	1.3 (1.6%)	2.3 (2.1%)
ΣE_{int}(π···π)	1.4 (2.7%)	2.5 (3%)	–	–	–	3.2 (3.6%)	7.3 (8.7%)	12.3 (11.1%)
ΣE_{int}(vdW)	8.2 (15.3%)	12.9 (15.7%)	5.3 (10.5%)	6.9 (8.6%)	2.8 (4.7%)	6.9 (7.8%)	8.1 (9.6%)	8.1 (7.4%)
B3LYP	fix.cell	opt.cell	fix.cell	opt.cell	fix.cell	opt.cell	fix.cell	opt.cell
E_{latt}(0K)	**51.0**	**82.2**	**50.4**	**80.5**	**54.6**	**88.1**	**73.5**	**116.5**
ΣE_{int}(N-H···N)	24.1 (47.2%)	33.9 (41.2%)	16.7 (33.2%)	22.8 (28.3%)	19.7 (36%)	25.1 (28.5%)	43.9 (59.7%)	50.7 (43.5%)
ΣE_{int}(N-H···C)	–	–	–	–	6.7 (12.3%)	10.7 (12.1%)	–	–
ΣE_{int}(C-H···X)	3.3 (6.4%)	6.1 (7.5%)	16.1 (32%)	16.2 (20.1%)	15.7 (28.8%)	21.4 (24.3%)	14.8 (20.1%)	38.6 (33.1%)
ΣE_{int}(C-H···π)	13.6 (26.7%)	25.8 (31.4%)	12.7 (25.3%)	34.9 (43.4%)	10 (18.2%)	14.7 (16.7%)	1.5 (2.0%)	2.8 (2.4%)
ΣE_{int}(π···π)	1.4 (2.8%)	2.6 (3.1%)	–	–	–	8.6 (9.7%)	5.6 (7.7%)	13.5 (11.6%)
ΣE_{int}(vdW)	8.6 (16.9%)	13.8 (16.7%)	4.8 (9.6%)	6.6 (8.2%)	2.6 (4.7%)	7.6 (8.7%)	7.7 (10.5%)	11.0 (9.4%)
PBE0	fix.cell	opt.cell	fix.cell	opt.cell	fix.cell	opt.cell	fix.cell	opt.cell
E_{latt}(0K)	**52.0**	**81.2**	**50.6**	**79.5**	**56.1**	**84.5**	**76.5**	**114.2**
ΣE_{int}(N-H···N)	25.5 (49%)	34.2 (42.1%)	24.8 (48.9%)	33.6 (42.2%)	20.9 (37.3%)	25.8 (30.5%)	47.3 (61.8%)	54.3 (47.5%)
ΣE_{int}(N-H···C)	–	–	–	–	6.8 (12.2%)	10.5 (12.5%)	–	–
ΣE_{int}(C-H···X)	3.1 (5.9%)	5.8 (7.1%)	8.1 (16.0%)	5.6 (7.0%)	16.0 (28.6%)	21.0 (24.9%)	14.7 (19.2%)	34.0 (29.8%)
ΣE_{int}(C-H···π)	13.8 (26.6%)	25.8 (31.7%)	12.8 (25.4%)	33.8 (42.5%)	9.8 (17.5%)	14.5 (17.1%)	1.4 (1.8%)	2.5 (2.2%)
ΣE_{int}(π···π)	1.4 (2.6%)	2.5 (3.0%)	–	–	–	8.1 (9.6%)	5.5 (7.2%)	12.8 (11.2%)
ΣE_{int}(vdW)	8.3 (15.9%)	13.0 (16.0%)	4.9 (9.7%)	6.6 (8.2%)	2.5 (4.4%)	4.5 (5.4%)	7.6 (10.0%)	10.6 (9.2%)
HSE06	fix.cell	opt.cell	fix.cell	opt.cell	fix.cell	opt.cell	fix.cell	opt.cell
E_{latt}(0K)	**52.0**	**80.0**	**50.8**	**78.1**	**56.3**	**83.2**	**79.1**	**113.3**
ΣE_{int}(N-H···N)	25.6 (49.2%)	34.2 (42.7%)	17.2 (33.8%)	22.5 (28.8%)	21.4 (38%)	26.1 (31.4%)	47.8 (60.4%)	54.7 (48.2%)
ΣE_{int}(N-H···C)	–	–	–	–	6.7 (11.8%)	10.2 (12.2%)	–	–
ΣE_{int}(C-H···X)	3.1 (5.9%)	5.6 (6.9%)	15.9 (31.2%)	16.2 (20.7%)	16.0 (28.5%)	25.4 (30.5%)	14.9 (18.9%)	33.5 (29.5%)
ΣE_{int}(C-H···π)	13.8 (26.5%)	25 (31.3%)	12.8 (25.2%)	32.8 (42.1%)	9.7 (17.2%)	14.2 (17%)	1.4 (1.8%)	2.4 (2.1%)
ΣE_{int}(π···π)	1.4 (2.6%)	2.4 (3.0%)	–	–	–	3.1 (3.7%)	7.2 (9.2%)	12.5 (11.0%)
ΣE_{int}(vdW)	8.2 (15.8%)	12.9 (16.1%)	5.0 (9.8%)	6.6 (8.4%)	2.5 (4.5%)	4.3 (5.2%)	7.7 (9.8%)	10.4 (9.2%)
CAM-B3LYP	fix.cell	opt.cell	fix.cell	opt.cell	fix.cell	opt.cell	fix.cell	opt.cell
E_{latt}(0K)	**50.5**	**77.0**	**49.2**	**78.7**	**53.8**	**86.7**	**72.2**	**112.3**
ΣE_{int}(N-H···N)	23.2 (46%)	31.0 (40.3%)	15.4 (31.3%)	20.4 (26.0%)	18.6 (34.7%)	23.1 (26.6%)	42.4 (58.7%)	48.7 (43.4%)
ΣE_{int}(N-H···C)	–	–	–	–	6.7 (12.5%)	10.0 (11.5%)	–	–
ΣE_{int}(C-H···X)	3.3 (6.5%)	5.9 (7.7%)	16.5 (33.5%)	15.6 (19.8%)	15.6 (29.0%)	24.4 (28.1%)	15.2 (21.0%)	37.7 (33.6%)
ΣE_{int}(C-H···π)	13.7 (27.2%)	24.8 (32.2%)	12.6 (25.6%)	33.3 (42.3%)	10.3 (19.1%)	14.2 (16.4%)	1.5 (2.1%)	2.5 (2.2%)
ΣE_{int}(π···π)	1.4 (2.8%)	2.4 (3.1%)	–	3.3 (4.2%)	–	8.1 (9.3%)	5.6 (7.7%)	13.0 (11.6%)
ΣE_{int}(vdW)	8.9 (17.6%)	12.9 (16.7%)	4.7 (9.6%)	6.1 (7.7%)	2.5 (4.6%)	7.0 (8.1%)	7.5 (10.4%)	10.4 (9.2%)

X = O, N

Table S10. Sublimation Gibbs energies, ΔG_{sub}^{298}, sublimation enthalpies, ΔH_{sub}^{298}, and fusion temperatures, T_{fus}, of compounds structurally related to aminopyridine isomers.

N	CAS	Name	ΔG_{sub}^{298} kJ·mol^{-1}	ΔH_{sub}^{298} kJ·mol^{-1}	T_{fus} K	Ref
1	99-92-3	4-aminoacetophenone	41.0	92.5	379.35	[1]
2	150-13-0	4-aminobenzoic acid	52.5	118.0	460.45	[2]
3	106-47-8	4-chloroaniline	25.5	80.5	343.65	[3]
4	1452-77-3	2-pyridinecarboxamide	35.3	91.3	379.55	[4]
5	98-92-0	Nicotinamide	49.3	111.7	402.65	[2]
6	1453-82-3	Isonicotinamide	49.1	117.0	429.85	[2]
7	99-09-2	3-nitroaniline	41.8	108.3	386.55	[5]
8	108-99-6	3-methylpyridine	9.4	62.2	255.01	[6]
9	591-27-5	3-aminophenol	41.8	105.4	394.95	[7]
10	123-30-8	4-aminophenol	46.6	109.7	460.05	[7]
11	95-54-5	1,2-diaminobenzene	32.3	85.5	375.25	[8]
12	108-45-2	1,3-diaminobenzene	35.0	90.4	339.15	[8]
13	106-50-3	1,4-diaminobenzene	37.5	92.2	414.25	[8]
14	106-49-0	4-aminotoluene	20.7	76.2	316.60	[9]
15	3676-85-5	4-aminophthalimide	72.3	142.4	567.15	[10]
16	35975-00-9	5-amino-6-nitroquinoline	68.2	136.4	545.15	[11]
17	580-17-6	3-aminoquinoline	42.4	103.1	364.65	[12]
18	611-34-7	5-aminoquinoline	43.7	105.0	383.15	[12]
19	580-15-4	6-aminoquinoline	43.8	105.7	387.15	[12]
20	578-66-5	8-aminoquinoline	33.2	93.3	343.15	[12]
21	60-09-3	4-aminoazobenzene	51.0	112.4	400.15	[13]
22	101-80-4	4,4'-diaminodiphenyl oxide	63.6	132.4	465.45	[14]
23	46492-08-4	benz[g]isoquinoline-5,10-dione	51.9	108.1	452.15	[15]
24	117-79-3	2-aminoanthraquinone	78.8	153.6	577.65	[10]
25	95-76-1	3,4-dichloro-Benzenamine	31.1	88.1	344.55	[3]
26	2243-62-1	1,5-Naphthalenediamine	55.5	120.2	469.55	[16]
27	2835-68-9	p-Aminobenzamide	61.7	131.2	455.55	[2]
28	2196-13-6	4-Pyridinecarbothioamide	56.0	118.8	475.95	[17]
29	5346-38-3	2-Pyridinecarbothioamide	38.3	87.3	407.05	[17]

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Table S11. Sublimation Gibbs energies, ΔG_{sub}^{298}, sublimation enthalpies, ΔH_{sub}^{298}, and fusion temperatures, T_{fus}, of compounds structurally related to 3-Hydroxypyridine.

N	CAS	Name	ΔG_{sub}^{298}	ΔH_{sub}^{298}	T_{fus}	Ref
			kJ·mol^{-1}	kJ·mol^{-1}	K	
1	90-15-3	1-naphthol	35.3	91.2	368.15	[1]
2	135-19-3	2-naphthol	38.2	94.2	394.60	[1]
3	108-46-3	1,3-dihydroxybenzene	37.7	94.7	382.55	[2]
4	123-31-9	1,4-dihydroxybenzene	43.8	103.9	445.55	[2]
5	533-73-3	1,2,3-trihydroxybenzene	53.4	124.2	413.25	[3]
6	87-66-1	1,2,3-trihydroxybenzene	42.7	103.9	405.65	[3]
7	108-73-6	1,3,5-trihydroxybenzene	69.4	135.5	491.85	[3]
8	95-71-6	Methylhydroquinone	39.0	101.9	399.65	[2]
9	2889-61-4	2,5-Dihydroxythiophenol	43.5	103.0	391.15	[2]
10	615-67-8	2-Chloro-1,4-dihydroxybenzene	35.7	99.7	381.15	[2]
11	583-69-7	2-Bromo-1,4-dihydroxybenzene	37.1	96.0	383.15	[2]
12	90-43-7	2-phenylphenol	32.2	88.5	333.75	[4]
13	92-69-3	4-phenylphenol	46.3	109.8	443.15	[4]
14	1806-29-7	2,2'-dihydroxybiphenyl	44.6	114.4	386.75	[4]
15	92-88-6	4,4'-dihydroxybiphenyl	69.4	143.0	560.75	[4]
16	576-24-9	2,3-dichlorophenol	22.5	76.9	330.05	[5]
17	120-83-2	2,4-dichlorophenol	21.6	78.0	318.15	[5]
18	95-77-2	3,4-dichlorophenol	29.7	89.8	339.65	[5]
19	106-41-2	4-bromophenol	27.3	84.2	337.85	[6]
20	108-43-0	3-chlorophenol	22.7	76.9	305.85	[5]
21	106-48-9	4-chlorophenol	23.8	77.1	316.90	[5]
22	100-02-7	4-nitrophenol	41.7	100.4	386.75	[7]
23	98-92-0	Nicotinamide	49.3	111.7	402.65	[8]
24	108-95-2	phenol	19.1	68.7	314.04	[9]
25	108-99-6	3-methylpyridine	9.4	62.2	255.01	[10]
26	108-89-4	4-methylpyridine	4.3	62.7	276.82	[10]
27	591-27-5	3-aminophenol	41.8	105.4	394.95	[11]
28	123-30-8	4-aminophenol	46.6	109.7	460.05	[11]
29	123-08-0	4-hydroxybenzaldehyde	41.4	98.2	390.15	[12]
30	95-48-7	2-methylphenol	19.5	76.0	304.18	[9]
31	106-44-5	4-methylphenol	21.7	73.9	307.92	[9]
32	150-76-5	4-methoxyphenol	30.0	88.5	328.45	[13]
33	123-07-9	4-ethylphenol	24.6	80.3	318.15	[14]
34	526-75-0	2,3-dimethylphenol	25.4	84.0	345.69	[14]
35	95-65-8	3,4-dimethylphenol	27.0	85.7	338.23	[14]
36	7640-33-7	7-bromo-5-chloro-8-hydroxyquinoline	49.5	113.2	450.65	[15]
37	521-74-4	5,7-dibromo-8-hydroxyquinoline	53.1	117.3	469.15	[15]
38	130-26-7	5-chloro-7-iodo-8-hydroxyquinoline	52.2	114.8	451.65	[15]
39	773-76-2	5,7-dichloro-8-hydroxyquinoline	47.0	109.3	452.65	[15]
40	83-73-8	5,7-diiodo-8-hydroxyquinoline	61.8	126.8	483.15	[15]
41	130-16-5	5-chloro-8-hydroxyquinoline	37.3	98.7	403.15	[15]
42	13207-63-1	5-iodo-8-hydroxyquinoline	49.7	121.3	399.15	[16]
43	4008-48-4	5-nitro-8-hydroxyquinoline	49.3	114.1	453.15	[17]
44	611-36-9	4-hydroxyquinoline	68.6	135.1	474.15	[18]
45	148-24-3	8-hydroxyquinoline	30.1	89.5	348.15	[17]
46	571-60-8	1,4-naphthohydroquinone	56.7	119.0	449.65	[19]
47	826-81-3	2-methyl-8-hydroxyquinoline	31.2	90.4	346.95	[17]
48	98-54-4	4-tert-butylphenol	30.1	85.9	373.25	[20]

49	66-71-7	1,10-phenanthroline	49.7	107.4	390.95	[21]
50	101-53-1	4-benzylphenol	41.6	97.1	358.25	[13]
51	81-60-7	1,4,5,8-tetrahydroxyanthraquinone	85.7	156.7	573.15	[22]
52	5315-79-7	1-hydroxypyrene	63.9	132.4	453.15	[23]
53	608-25-3	2-Methylresorcinol	36.3	99.2	390.05	[24]
54	496-73-1	4-Methylresorcinol	39.0	107.3	379.15	[24]
55	609-70-1	4-Hydroxynicotinic Acid	78.8	148.1	532.75	[25]
56	27828-71-3	5-Hydroxynicotinic Acid	80.6	149.8	571.45	[25]
57	230-07-9	4,7-Phenanthroline	50.9	118.4	445.50	[21]
58	371-41-5	4-Fluorophenol	19.9	74.1	320.45	[6]
59	90-01-7	2-Hydroxymethylphenol	34.3	99.5	357.15	[26]
60	540-38-5	4-Iodophenol	32.3	90.2	365.85	[6]
61	831-82-3	4-Phenoxyphenol	43.2	112.8	356.75	[27]
62	93-60-7	methyl nicotinate	22.3	80.1	312.65	[28]
63	114-33-0	N-methylnicotinamide	44.2	107.4	379.15	[29]
64	6972-69-6	N,N-dimethylnicotinamide	33.3	94.0	317.35	[29]
65	2417-10-9	2-hydroxy-diphenyl ether	36.5	92.3	375.35	[30]
66	89-00-9	Pyridine-2,3-dicarboxylic acid	55.1	128.7	456.05	[31]

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Table S12. Sublimation Gibbs energies, ΔG_{sub}^{298}, sublimation enthalpies, ΔH_{sub}^{298}, and fusion temperatures, T_{fus}, of compounds structurally related to 2-(1H-Imidazol-2-yl)pyridine.

N	CAS	Name	ΔG_{sub}^{298} kJ·mol^{-1}	ΔH_{sub}^{298} kJ·mol^{-1}	T_{fus} K	Ref
1	4394-00-7	Niflumic acid	61.3	130.2	478.95	[1]
2	288-32-4	imidazole	31.7	83.1	362.82	[2]
3	1072-62-4	2-ethylimidazole	34.6	89.6	352.65	[3]
4	1452-77-3	Picolinamide	35.3	91.3	379.55	[4]
5	98-92-0	Nicotinamide	49.3	111.7	402.65	[5]
6	1453-82-3	Isonicotinamide	49.1	117.0	429.85	[5]
7	51-17-2	benzimidazole	47.2	102.2	443.25	[2]
8	27032-01-5	pyridinium dicyanomethylide	67.9	128.7	518.15	[6]
9	120-72-9	indole	27.5	75.0	325.65	[7]
10	7640-33-7	7-bromo-5-chloro-8-hydroxyquinoline	49.5	113.2	450.65	[8]
11	521-74-4	5,7-dibromo-8-hydroxyquinoline	53.1	117.3	469.15	[8]
12	130-26-7	5-chloro-7-iodo-8-hydroxyquinoline	52.2	114.8	451.65	[8]
13	773-76-2	5,7-dichloro-8-hydroxyquinoline	47.0	109.3	452.65	[8]
14	83-73-8	5,7-diiodo-8-hydroxyquinoline	61.8	126.8	483.15	[8]
15	130-16-5	5-chloro-8-hydroxyquinoline	37.3	98.7	403.15	[8]
16	13207-63-1	5-iodo-8-hydroxyquinoline	49.7	121.3	399.15	[9]
17	607-34-1	5-nitroquinoline	36.2	94.2	347.15	[10]
18	613-50-3	6-nitroquinoline	43.8	103.8	426.65	[10]
19	607-35-2	8-nitroquinoline	44.8	106.7	363.15	[10]
20	4008-48-4	5-nitro-8-hydroxyquinoline	49.3	114.1	453.15	[11]
21	148-24-3	8-hydroxyquinoline	30.1	89.5	348.15	[11]
22	35975-00-9	5-amino-6-nitroquinoline	68.2	136.4	545.15	[12]
23	611-34-7	5-aminoquinoline	43.7	105.0	383.15	[13]
24	580-15-4	6-aminoquinoline	43.8	105.7	387.15	[13]
25	578-66-5	8-aminoquinoline	33.2	93.3	343.15	[13]
26	83-34-1	3-methylindole	30.4	83.3	370.65	[7]
27	1436-43-7	2-cyanoquinoline	37.3	94.4	368.15	[14]
28	3138-86-1	2,3-bis(bromomethyl)quinoxaline	49.3	114.0	423.64	[15]
29	881-07-2	8-nitroquinaldine	47.4	111.0	413.15	[10]
30	826-81-3	2-methyl-8-hydroxyquinoline	31.2	90.4	346.95	[11]
31	2379-55-7	2,3-dimethylquinoxaline	31.3	87.8	379.49	[15]
32	66-71-7	1,10-phenanthroline	49.7	107.4	390.95	[16]
33	46492-08-4	benz[g]isoquinoline-5,10-dione	51.9	108.1	452.15	[17]
34	229-87-8	Phenanthridine	42.2	100.1	379.74	[17]
35	612-96-4	2-phenylquinoline	44.3	105.4	359.15	[18]
36	670-96-2	2-phenyl-1H-Imidazole	50.1	113.6	418.15	[19]
37	244-63-3	9H-pyrido[3,4-b]indole	59.3	116.3	480.15	[20]
38	15827-72-2	2,5-Diphenylpyridine	56.8	123.7	444.30	[21]
39	92-07-9	3,5-Diphenylpyridine	56.1	129.3	409.25	[21]
40	609-71-2	2-Hydroxynicotinic Acid	71.6	128.3	534.30	[22]
41	230-07-9	4,7-Phenanthroline	50.9	118.4	445.50	[16].
42	230-46-6	1,7-Phenanthroline	42.8	114.2	351.75	[16]
43	2459_07-6	methyl picolinate	24.0	81.8	289.25	[23]
44	93-60-7	methyl nicotinate	22.3	80.1	312.65	[24]
45	114-33-0	N-methylnicotinamide	44.2	107.4	379.15	[24]
46	6972-69-6	N,N-dimethylnicotinamide	33.3	94.0	317.35	[24]
47	54-85-3	Isoniazid	49.5	101.0	446.25	[25]

48	2196-13-6	4-Pyridinecarbothioamide	56.0	118.8	475.95	[25]
49	5346-38-3	2-Pyridinecarbothioamide	38.3	87.3	407.05	[25]
50	not	N-(2-chloro-3-pyridinyl)-benzenesulfonamide	56.7	115.0	426.25	[5]
51	499-83-2	Dipicolinic acid	68.6	134.3	528.05	[26]
52	36947-68-9	2-isopropylimidazole	36.2	92.2	403.15	[27]
53	89-00-9	Quinolinic acid	55.1	128.7	456.05	[26]

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Table S13. Coefficients of the correlation equation (31) for the clusters including the considered compound as a one from the components of the two-component crystal.

№	CF1	CF1:CF2	A	B	R^a	σ^b	n^c	T_{fus} /°C
1	Caffeine	1:1	132±21	0.673±0.045	0.9512	16.00	26	236.1
	Caffeine	2:1	223±30	0.445±0.063	0.9623	10.20	6	236.1
2	Carbamazepine	1:1	245±15	0.415±0.032	0.8990	11.50	42	164.0
	Carbamazepine	2:1	275±61	0.369±0.142	0.6544	18.30	11	164.0
3	Isoniazid	1:1	195±23	0.495±0.052	0.8782	14.50	29	173.1
	Isoniazid	2:1	271±30	0.316±0.063	0.8582	12.80	11	173.1
4	Isonicotinamide	1:1	243±26	0.420±0.059	0.7533	21.90	41	156.7
	Isonicotinamide	2:1	265±23	0.400±0.051	0.8919	14.30	18	156.7
	Isonicotinamide	1:2	220±27	0.513±0.064	0.9704	7.36	6	156.7
5	Nicotinamide	1:1	178±15	0.514±0.033	0.8936	15.60	63	129.5
	Nicotinamide	1:2	-73±71	1.086±0.151	0.9381	16.80	9	129.5
	Nicotinamide	2:1	268±28	0.322±0.058	0.8907	14.30	10	129.5

[a] Pair correlation coefficient;
[b] Standard deviation;
[c] A number of points in the cluster;