

Two models to estimation the density of organiccocrystals

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Table S1 the systematic name of the components of the cocrystals

abbreviate	Systematic name
CL-20	2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane
TNT	2,4,6-trinitrotoluene
DNG	3,5-dinitro-3,5-diazaheptane
MTNP	1-methyl-3,4,5-trinitro-1H-pyrazole
AZ2	tris[1,2,5]oxadiazolo[3,4-b:3',4'-d:3'',4''-f]azepin-7-amine
NEX-1	1-methyl-3,5-dinitro-1,2,4-triazole
GTA	propane-1,2,3-triyl triacetate
TODAAZ	7H-tris[1,2,5]oxadiazolo[3,4-b:3',4'-d:3'',4''-f]azepine
NFQN	1,4-Naphthoquinone
BQN	b-benzoquinone
DNB	1,3-dinitrobenzene
DNDAP	N,N'-dimethyl-N,N'-dinitromethanediamine
4,5-MDNI	1-methyl-4,5-dinitro-1H-imidazole
HMX	1,3,5,7-Tetranitro-1,3,5,7-tetra-azacyclo-octane
FA	4-fluoroaniline
DAT	4-methylbenzene-1,3-diamine
NMP	N-methyl-2-pyrrolidinone
PDCA	piperazine-1,4-dicarbaldehyde
PNO	pyridine N-oxide

BTF	benzotrifuroxan
TNB	1,3,5-trinitrobenzene
MATNB	N-methyl-2,4,6-trinitroaniline
TNAZ	1,3,3-trinitroazetidine
TNA	2,4,6-trinitroaniline
TNT	2,4,6-trinitrotoluene
NNAP	2-Methyl-1,3,5-trinitrobenzene 1-nitronaphthalene
1-BN	1-bromonaphthalene
Ant	anthracene
9-BN	9-bromoanthracene
Per	perylene
T2	thieno[3,2-b]thiophene
DMDBT	4,6-dimethyldibenzothiophene
PDA	1,2-phenylenediamine
DMB	1,4-dimethoxybenzene
TNB	2-methyl-1,3,5-trinitrobenzene
ABA	2-Aminobenzoic acid
PA	10H-Phenothiazine
NAP	naphthalene
Phe	phenanthrene
TTF	tetrathiafulvalene
EDNA	N,N'-dinitroethane-1,2-diamine
BPY	4,4'-bipyridine
DPYETA	4,4'-ethane-1,2-diyl dipyridine
DPYETE	4,4'-ethene-1,2-diyl dipyridine
PYDOXD	pyrazine N,N'-dioxide
DNDAP	N,N'-dimethyl-N,N'-dinitromethanedia mine
FTDO	[1,2,5]oxadiazolo[3,4-e][1,2,3,4]tetrazine 4,6-dioxide

DADP	3,3,6,6-tetramethyl-1,2,4,5-tetroxane
TBTNB	1,3,5-Tribromo-2,4,6-trinitrobenzene
TCTNB	1,3,5-Trichloro-2,4,6-trinitrobenzene
TITNB	1,3,5-triiodo-2,4,6-trinitrobenzene
DNBT	5,5'-dinitro-2H,2'H-3,3'-bi-1,2,4-triazole
DZDBT	4,4'-diazenediylbis(4H-1,2,4-triazole)
DNPP	3,6-dinitro-1,4-dihydropyrazolo[4,3-c]pyrazole
Organic cocrystal	
NNAP	1-nitronaphthalene
TNP	2,4,6-trinitrophenol
MACIC	Methyl 5-amino-4-carbamoyl-1H-imidazole-1-carboxylate
TZM	temozolomide
DHDS	2,3-dihydroxysuccinate
TZM	Temozolomide
DNBZA	3,5-Dinitrobenzoic acid
NA	nicotinic acid
MBD	3-methylbenzene-1,2-diamine
MTNB	2-methyl-1,3,5-trinitrobenzene
PM	2,4,6(1H,3H,5H)-Pyrimidinetrione
MC	Myricetin
PC	piracetam
AB	1,3,5-tris(4-aminophenyl)benzene
MTNB	2-methyl-1,3,5-trinitrobenzene
NDT	5-Nitro-2,4-dihydro-3H-1,2,4-triazol-3-one
THTZT	5,6,7,8-tetrahydrotetrazolo[1,5-b][1,2,4]triazine
IDT	1-Isopropyl-3,5-dinitro-1H-1,2,4-triazole
NTZ	3-nitro-1H-1,2,4-triazole
DNBA	3,5-Dinitrobenzoic acid 4-(dimethylamino)
BA	benzoic acid

PZ	Pyrazine
OA	oxalic acid
TNP	2,4,6-Trinitrophenol
MDNI	1-methyl-2,4-dinitro-1H-imidazole
DNBA	3,5-dinitrobenzoic acid
TA	4H-1,2,4-triazol-4-amine
NMI	4-Nitro-5-methoxy-1H-imidazole
NMI	5-nitro-4-methoxy-1H-imidazole
AN	Adenine
HP	hydrogen peroxide
NF	Nitrofurantoin
CA	citric acid
NF	Nitrofurantoin
UREA	urea
NPO	4-nitropyridine-N-oxide
PA	picric acid
CA	cyanuric acid
PZCX	Pyrazine-2-carboxamide
DHXBED	3,4-dihydroxycyclo but-3-ene-1,2-dione
TNP	2,4,6-Trinitrophenol
TAD	1,3,5,7-tetra-azatricyclo[3.3.1.1 ^{3,7}]decane
IZO	Imidazolidin-2-one
	3,4,5-trihydroxybenzoic acid p-Nitropyridine-N-oxide
DLTA	DL-tartaric acid
LTA	L-tartaric acid
DNBZA	3,5-dinitrobenzoic acid
TZ	1H-1,2,3-triazole
OA	oxalic acid
PZCX	pyrazine-2-carboxamide

OA	oxalic acid
TZA	2H-Tetrazol-2-amine
NDTZI	N-nitro-1,4-dihydro-5H-tetrazol-5-imine
TZTM	1,3,5-triazine-2,4,6-triamine
HP	hydrogen peroxide
BM	Benzamide
TNP	2,4,6-trinitrophenol

Table S2 the three input parameters and one output parameter used in ANN model^a

No	Co-formers	Refcode	MS	RTm	E1u	ΔE_{hb}	ρ_1	ρ_2	ρ_{exp}
1	CL-20:TNT	IZUZUZ	3.830	20.000	0.479	-6.229	1.916	1.564	1.911
2	CL-20:DNG	JABYOD	3.645	18.009	0.517	-15.978	1.916	1.547	1.750
3	CL-20:MTNP	QAPNAZ	3.935	20.648	0.555	-8.774	1.916	1.784	1.932
4	CL-20:AZ2	TETTAQ	3.245	20.366	0.476	-11.568	1.916	1.808	1.939
5	CL-20:NEX-1	WEPGEG	3.825	18.374	0.493	-13.194	1.916	1.673	1.882
6	CL-20:GTA	XAQFUS	3.495	17.449	0.466	-22.712	1.916	1.155	1.650
7	CL-20:TODAAZ	HIVGAW	3.215	21.240	0.476	-3.540	1.916	1.871	1.971
8	CL-20:NFQN	ROSMIX	3.295	17.656	0.522	-17.230	1.916	1.417	1.774
9	CL-20:BQN	ROSMOD	3.520	16.963	0.467	-12.186	1.916	1.325	1.737
10	CL-20:DNB	TIVJUF	3.740	18.933	0.490	-10.910	1.916	1.569	1.880
11	CL-20:4,5-MDNI	NILCIX	3.780	19.108	0.533	-21.335	1.916	1.637	1.882
12	HMX:PNO	WEPTAP	3.305	10.105	0.452	-18.111	1.840	1.358	1.700
13	HMX:FA	ZEZHET	3.355	7.763	0.488	-1.407	1.840	1.400	1.687
14	HMX:PDCA	ZEZGOC	3.295	8.035	0.444	-13.482	1.840	1.400	1.630
15	BTF:TNA	ZEVNUL	3.655	17.002	0.475	-1.661	1.862	1.901	1.811
16	BTF:TNB	GEXMED	3.535	17.199	0.485	-3.752	1.676	1.901	1.806
17	BTF:MATNB	GEXMON	3.430	16.290	0.489	-3.122	1.643	1.901	1.804
18	BTF:TNA	GEXMIH	3.530	17.271	0.484	-3.573	1.773	1.901	1.884

19	TNT: NNAP	TOZMUS	3.295	12.456	0.497	-10.948	1.564	1.564	1.539
20	TNT:1-BN	URIJAH	2.940	14.478	0.494	-3.000	1.564	1.480	1.737
21	TNT:Ant	URIJEL	2.900	11.298	0.493	-3.156	1.564	1.240	1.515
22	TNT:9-BN	URIJIP	2.920	13.754	0.493	-3.079	1.564	1.592	1.688
23	TNT:Per	URIJUB	2.830	9.067	0.529	-3.070	1.564	1.311	1.531
24	TNT:T2	URIKEM	2.890	13.508	0.501	-3.626	1.564	1.542	1.677
25	TNT:DMDBT	URIKUC	2.880	10.555	0.540	-3.469	1.564	1.299	1.496
26	TNT:PDA	URILAJ	3.160	9.832	0.509	-5.745	1.564	1.214	1.578
27	TNT:DMB	URILEN	3.065	9.944	0.475	-9.987	1.564	1.231	1.501
28	TNT:TNB	NIBJUF	3.915	15.532	0.449	-3.547	1.564	1.676	1.640
29	ABA:TNT	URILUD	3.395	8.767	0.488	-6.917	1.564	1.362	1.594
30	MACIC:TZM	ACERAD	3.075	5.538	0.530	-5.505	1.622	1.448	1.605
31	DHDS:TZM	ACETEJ	3.690	6.970	0.503	-39.198	1.821	1.622	1.625
32	DNBZA:NA	AWUDEB	3.440	9.204	0.491	-16.189	1.683	1.473	1.607
33	MBD:MTNB	DIFZOK	3.115	9.764	0.475	-5.664	1.564	1.148	1.522
34	PM:UREA	EFOZAB03	3.890	3.799	0.553	-23.672	1.589	1.335	1.644
35	MC:PC	FIXROV01	3.050	7.521	0.578	-17.990	1.711	1.470	1.606
36	AB:MTNB	FONHOH	3.005	11.972	0.426	-6.309	1.564	1.250	1.442
37	NDT:THTZT	FOYSUJ	3.055	7.189	0.521	-22.546	1.577	1.919	1.664
38	IDT:NTZ	FUFSOQ	3.500	8.734	0.544	-11.249	1.542	1.797	1.644
39	DNBA:BA	GAUTAM15	3.255	8.004	0.493	-22.893	1.683	1.040	1.697
40	PZ:OA	GUDSUV	3.610	4.676	0.594	-17.531	1.252	1.653	1.609
41	TNP:MDNI	HARJOB	3.865	11.143	0.500	-8.721	1.760	1.637	1.769
42	DNBA:TA	IJAKAH	3.255	8.744	0.509	-36.695	1.673	1.544	1.635
43	NMI:NMI	ITIXUE	3.230	5.235	0.564	-16.332	1.660	1.660	1.660
44	AN:HP	JOZZED	4.225	3.923	0.661	-2.994	1.494	1.130	1.614
45	NF:CA	LEWTAK	3.710	8.966	0.516	-3.523	1.642	1.542	1.627
46	NF:UREA	ORUXUV	3.710	5.487	0.597	-5.895	1.642	1.335	1.661

47	NPO:PA	OWIYEZ	3.755	11.283	0.474	-72.061	1.771	1.551	1.682
48	UREA:CA	PANVUV	3.945	5.265	0.527	-29.511	1.818	1.319	1.672
49	PZCX:DHXBED	PAQNOM	3.505	5.901	0.574	-16.919	1.441	1.906	1.628
50	DNPA:ODADA	QARQUY	3.430	8.233	0.516	-8.733	1.900	1.608	1.775
51	TNP:TAD	QONYUP	2.870	9.880	0.509	-18.529	1.345	1.771	1.685
52	IZO:DLTA	RUWPEG	3.540	7.075	0.490	-9.258	1.863	1.637	1.656
53	IZO:LTA	UHACIQ	3.590	5.519	0.455	-33.493	1.760	1.496	1.631
54	IZO:LTA	UHAFEP	3.590	5.338	0.453	-27.322	1.760	1.496	1.607
55	DNBZA:TZ	UNAWUD	3.170	7.800	0.464	-27.865	1.688	1.274	1.640
56	Urea:OA	UROXAM	4.530	3.099	0.589	-28.110	1.391	1.653	1.679
57	PZCX:OA	UZODUK	3.910	6.013	0.574	-31.306	1.301	1.653	1.628
58	TZA:NDTZI	VAZBIJ	3.175	6.290	0.581	-12.882	1.867	1.711	1.790
59	TZTM:HP	YAFFUJ	4.445	3.335	0.639	-5.759	1.578	1.130	1.636
60	BM:TNP	YUQHEY	3.370	9.626	0.511	-23.115	1.771	1.341	1.632

^aAll energies are in $\text{kJ}\cdot\text{mol}^{-1}$, and the density are $\text{g}\cdot\text{cm}^{-3}$

Table S3 the calculation values of the application parameters of 60 organic cocrystals in surface electrostatic potential correction model^a

No	Co-formers	Refcode	M	V _m	M/V _m	$u\sigma_{\text{tot}}^2$
1	CL-20:TNT	IZUZUZ	665.317	494.381	1.346	42.877
2	CL-20:DNG	JABYOD	630.359	487.270	1.294	71.885
3	CL-20:MTNP	QAPNAZ	655.282	475.234	1.379	28.317
4	CL-20:AZ2	TETTAQ	672.320	492.017	1.366	45.318
5	CL-20:NEX-1	WEPGEG	611.273	442.439	1.382	51.585
6	CL-20:GTA	XAQFUS	640.390	512.960	1.248	52.013
7	CL-2:TODAAZ	HIVGAW	657.305	477.701	1.376	26.430
8	CL-20:NFQN	ROSMIX	596.341	453.807	1.314	32.426
9	CL-20:BQN	ROSMOD	546.281	407.602	1.340	28.135
10	CL-20:DNB	TIVJUF	606.293	447.782	1.354	38.624
11	CL-20:4,5-MDNI	NILCIX	610.285	456.074	1.338	51.220
12	HMX:PNO	WEPTAP	391.256	326.290	1.199	59.024
13	HMX:FA	ZEZHET	407.274	331.698	1.228	79.057
14	HMX:PDCA	ZEZGOC	438.312	367.847	1.192	72.889
15	BTF:TNA	ZEVNUL	444.189	325.019	1.367	42.638
16	BTF:TNB	GEXMED	465.207	350.830	1.326	27.475
17	BTF:MATNB	GEXMON	494.248	379.013	1.304	44.083
18	BTF:TNA	GEXMIH	480.222	363.992	1.319	36.075
19	TNT: NNAP	TOZMUS	400.302	349.462	1.145	37.773
20	TNT:1-BN	URIJAH	434.201	347.532	1.249	31.624

21	TNT:Ant	URIJEL	404.357	369.656	1.094	26.991
22	TNT:9-BN	URIJIP	484.261	395.686	1.224	31.301
23	TNT:Per	URIJUB	467.352	435.783	1.072	26.575
24	TNT:T2	URIKEM	335.289	309.591	1.083	33.081
25	TNT:DMDBT	URIKUC	431.363	401.162	1.075	26.426
26	TNT:PDA	URILAJ	341.275	299.556	1.139	43.138
27	TNT:DMB	URILEN	365.297	328.383	1.112	26.551
28	TNT:TNB	NIBJUF	440.236	350.818	1.255	27.936
29	ABA:TNT	URILUD	364.269	316.820	1.150	43.636
30	MACIC:TZM	ACERAD	378.308	337.922	1.120	79.727
31	DHDS:TZM	ACETEJ	344.239	298.148	1.155	91.560
32	DNBZA:NA	AWUDEB	335.227	292.450	1.146	47.423
33	MBD:MTNB	DIFZOK	349.302	314.464	1.111	37.573
34	PM:UREA	EFOZAB03	188.142	177.199	1.062	112.646
35	MC:PC	FIXROV01	460.393	413.366	1.114	77.310
36	AB:MTNB	FONHOH	578.582	558.455	1.036	42.179
37	NDT:THTZT	FOYSUJ	256.185	221.151	1.158	119.776
38	IDT:NTZ	FUFSOQ	315.205	270.372	1.166	85.818
39	DNBA:BA	GAUTAM15	377.308	353.839	1.066	67.940
40	PZ:OA	GUDSUV	170.123	157.037	1.083	73.612
41	TNP:MDNI	HARJOB	401.203	323.240	1.241	58.591
42	DNBA:TA	IJAKAH	296.198	256.505	1.155	116.112
43	NMI:NMI	ITIXUE	286.203	250.608	1.142	122.746

44	AN:HP	JOZZED	169.143	156.496	1.081	81.846
45	NF:CA	LEWTAK	430.281	368.545	1.168	70.276
46	NF:UREA	ORUXUV	298.214	261.793	1.139	168.265
47	NPO:PA	OWIYEZ	369.201	299.918	1.231	49.926
48	UREA:CA	PANVUV	189.130	164.253	1.151	125.835
49	PZCX:DHXBED	PAQNOM	237.170	209.957	1.130	111.549
50	DNPA:ODADA	QARQUY	273.168	228.040	1.198	80.010
51	TNP:TAD	QONYUP	369.293	319.139	1.157	60.385
52	IZO:DLTA	RUWPEG	310.217	271.487	1.143	75.169
53	IZO:LTA	UHACIQ	236.179	211.730	1.115	81.321
54	IZO:LTA	UHAFEP	236.179	213.956	1.104	129.745
55	DNBZA:TZ	UNAWUD	281.183	239.904	1.172	99.303
56	Urea:OA	UROXAM	150.089	133.287	1.126	199.894
57	PZCX:OA	UZODUK	213.148	194.640	1.095	116.026
58	TZA:NDTZI	VAZBIJ	215.137	181.666	1.184	103.862
59	TZTM:HP	YAFFUJ	160.136	149.606	1.070	72.411
60	BM:TNP	YUQHEY	350.242	303.406	1.154	59.682

^a*M* are in g·mol⁻¹, the *V_m* are in Å³ and the *υσ_{tot}*² are in (kcal·mol)²