Electronic supplementary information for:

Two crystal forms of 4′-methyl-2,4-dinitrodiphenylamine: polymorphism governed by conformational flexibility of a supramolecular synthon

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1. Fragments of crystal packing of polymorphic forms I and II

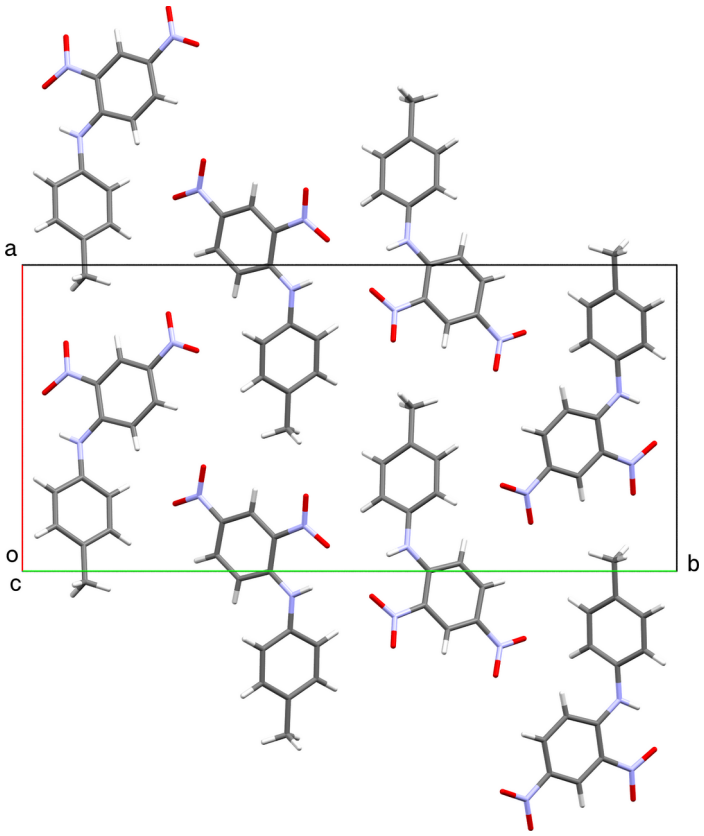

Figure. S1. Fragment of crystal packing of the polymorph **I**, view along the crystallographic *c* axis.

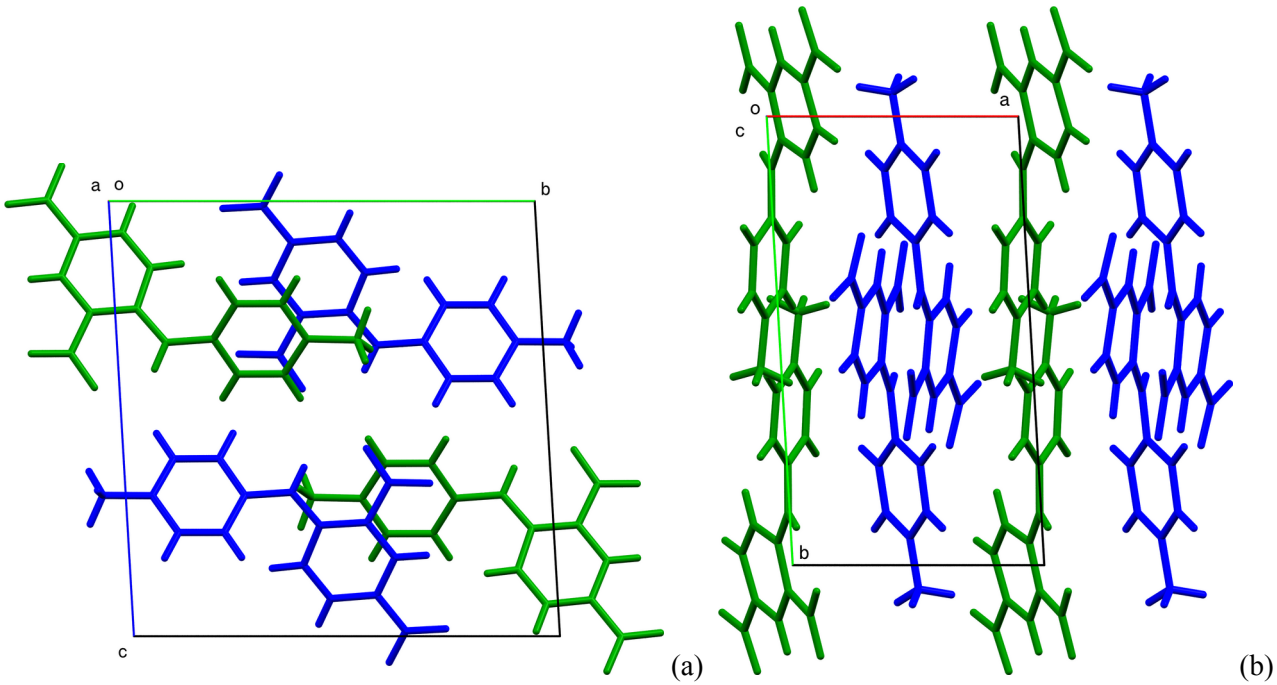

Figure. S2. Fragments of crystal packing of the polymorph **II**, view along the crystallographic *a* axis (a) and along the crystallographic *c* axis (b). The crystallographically independent molecules are shown in blue and green.

2. Crystal structure of the form I, in CIF format, optimized by PBE0-D3/POB-TZVP method

Listing S1: Coordinates of form **I** optimized by PBE0-D3/POB-TZVP method

```
data_1a-pbe0d3
_symmetry_cell_setting           orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 2'
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 1/2+x,1/2-y,-z
4 1/2-x,1/2+y,-z
_cell_length_a                   12.2141
_cell_length_b                   26.1179
_cell_length_c                   3.8006
_cell_angle_alpha                90.000
_cell_angle_beta                 90.000
_cell_angle_gamma                90.000
_cell_volume                     1212.42
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_thermal_displace_type
O1 O 0.08367 0.46083 0.18102 0.0300 Uiso
O2 O 0.2475 0.42557 0.1876 0.0300 Uiso
O3 O 0.32266 0.27108 0.76135 0.0300 Uiso
O4 O 0.19158 0.23072 1.0521 0.0300 Uiso
N1 N 0.14786 0.42454 0.26733 0.0300 Uiso
N2 N 0.22441 0.26648 0.85634 0.0300 Uiso
N3 N -0.08245 0.41251 0.44535 0.0300 Uiso
H3N H -0.05158 0.44475 0.33521 0.0300 Uiso
C1 C -0.00851 0.37721 0.53507 0.0300 Uiso
C2 C 0.10529 0.38215 0.45414 0.0300 Uiso
C3 C 0.18053 0.34517 0.55533 0.0300 Uiso
H3A H 0.26576 0.35033 0.48966 0.0300 Uiso
C4 C 0.1459 0.30332 0.74188 0.0300 Uiso
C5 C 0.03471 0.29681 0.82555 0.0300 Uiso
H5A H 0.00843 0.26369 0.97395 0.0300 Uiso
C6 C -0.03946 0.3323 0.72136 0.0300 Uiso
H6A H -0.1251 0.32686 0.78161 0.0300 Uiso
C7 C -0.19576 0.4114 0.53165 0.0300 Uiso
C8 C -0.23899 0.4523 0.71794 0.0300 Uiso
H8A H -0.18651 0.48335 0.80293 0.0300 Uiso
C9 C -0.34829 0.45187 0.80687 0.0300 Uiso
H9A H -0.3803 0.48254 0.96974 0.0300 Uiso
C10 C -0.41599 0.41152 0.70926 0.0300 Uiso
C11 C -0.37137 0.3717 0.51508 0.0300 Uiso
H11A H -0.42295 0.34015 0.43204 0.0300 Uiso
C12 C -0.26191 0.37135 0.42493 0.0300 Uiso
H12A H -0.22892 0.34026 0.26996 0.0300 Uiso
C13 C -0.53382 0.41121 0.81424 0.0300 Uiso
H13A H -0.57222 0.37457 0.75425 0.0300 Uiso
H13B H -0.58032 0.44142 0.68294 0.0300 Uiso
H13C H -0.54192 0.41761 1.0963 0.0300 Uiso
```

3. Crystal structure 1b, in CIF format, optimized by PBE0-D3/POB-TZVP method

Listing S2: Coordinates of form **II** optimized by PBE0-D3/POB-TZVP method

```
data_1b-pbe0d3
_symmetry_cell_setting           triclinic
_symmetry_space_group_name_H-M   'P -1'
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                   7.1979
_cell_length_b                   12.8243
_cell_length_c                   13.1514
_cell_angle_alpha                86.287
_cell_angle_beta                 83.627
_cell_angle_gamma                86.296
_cell_volume                     1201.93
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_thermal_displace_type
O1 O 0.49069 -0.43033 -0.42451 0.0300 Uiso
O2 O 0.47931 -0.28499 -0.34296 0.0300 Uiso
O3 O 0.65136 -0.27661 -0.01119 0.0300 Uiso
O4 O 0.75707 -0.42102 0.06959 0.0300 Uiso
N1 N 0.51 -0.38193 -0.34541 0.0300 Uiso
N2 N 0.69349 -0.37368 -0.00736 0.0300 Uiso
N3 N 0.57432 -0.60995 -0.33131 0.0300 Uiso
H3N H 0.54192 -0.56996 -0.39684 0.0300 Uiso
C1 C 0.60419 -0.55123 -0.25498 0.0300 Uiso
C2 C 0.57104 -0.44006 -0.25835 0.0300 Uiso
C3 C 0.59766 -0.38286 -0.17619 0.0300 Uiso
H3 H 0.56364 -0.29956 -0.1801 0.0300 Uiso
C4 C 0.66596 -0.43261 -0.09135 0.0300 Uiso
C5 C 0.71096 -0.54081 -0.08729 0.0300 Uiso
H5 H 0.77135 -0.57831 -0.02177 0.0300 Uiso
C6 C 0.67751 -0.59777 -0.16592 0.0300 Uiso
H6 H 0.71077 -0.68109 -0.16232 0.0300 Uiso
C7 C 0.57287 -0.7208 -0.32748 0.0300 Uiso
C8 C 0.64924 -0.77239 -0.41309 0.0300 Uiso
H8 H 0.71933 -0.72906 -0.47808 0.0300 Uiso
C9 C 0.63236 -0.87902 -0.41508 0.0300 Uiso
H9 H 0.6877 -0.9191 -0.48291 0.0300 Uiso
C10 C 0.54374 -0.93598 -0.33216 0.0300 Uiso
C11 C 0.47298 -0.88291 -0.24601 0.0300 Uiso
H11 H 0.40138 -0.9261 -0.18118 0.0300 Uiso
C12 C 0.48284 -0.77604 -0.24379 0.0300 Uiso
H12 H 0.41593 -0.73513 -0.17872 0.0300 Uiso
C13 C 0.51901 -1.05039 -0.33599 0.0300 Uiso
H13A H 0.58596 -1.08148 -0.40696 0.0300 Uiso
H13B H 0.37104 -1.06657 -0.3297 0.0300 Uiso
H13C H 0.57601 -1.09462 -0.27176 0.0300 Uiso
O1' O 0.08866 0.05314 -0.42466 0.0300 Uiso
O2' O 0.08666 0.19764 -0.34273 0.0300 Uiso
O3' O -0.16816 0.22333 -0.00222 0.0300 Uiso
O4' O -0.27587 0.08445 0.08844 0.0300 Uiso
N1' N 0.05237 0.10329 -0.34396 0.0300 Uiso
N2' N -0.20457 0.12812 0.00598 0.0300 Uiso
N3' N -0.01422 -0.1205 -0.32526 0.0300 Uiso
H3N' H 0.02373 -0.08286 -0.39385 0.0300 Uiso
C1' C -0.0619 -0.05844 -0.24747 0.0300 Uiso
C2' C -0.03035 0.05069 -0.2536 0.0300 Uiso
C3' C -0.07586 0.1108 -0.16983 0.0300 Uiso
H3' H -0.0411 0.19175 -0.17604 0.0300 Uiso
C4' C -0.16079 0.06645 -0.08032 0.0300 Uiso
C5' C -0.2044 -0.03897 -0.07304 0.0300 Uiso
H5' H -0.2779 -0.07196 -0.00345 0.0300 Uiso
C6' C -0.15339 -0.09918 -0.15359 0.0300 Uiso
H6' H -0.18719 -0.18024 -0.14738 0.0300 Uiso
C7' C -0.00663 -0.23136 -0.3192 0.0300 Uiso
C8' C -0.06185 -0.28257 -0.39975 0.0300 Uiso
H8' H -0.11947 -0.23807 -0.46306 0.0300 Uiso
C9' C -0.04002 -0.39048 -0.39891 0.0300 Uiso
H9' H -0.08288 -0.42979 -0.46221 0.0300 Uiso
C10' C 0.03272 -0.44924 -0.31828 0.0300 Uiso
C11' C 0.08216 -0.39644 -0.23735 0.0300 Uiso
H11' H 0.14034 -0.44057 -0.17405 0.0300 Uiso
C12' C 0.06627 -0.28845 -0.23797 0.0300 Uiso
H12' H 0.11654 -0.24878 -0.17696 0.0300 Uiso
C13' C 0.0656 -0.5654 -0.32051 0.0300 Uiso
H13C H 0.07227 -0.6017 -0.24371 0.0300 Uiso
H13D H 0.19851 -0.58629 -0.36503 0.0300 Uiso
H13E H -0.04261 -0.60116 -0.35584 0.0300 Uiso
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4. List of bond critical points in polymorphs I and II.

The sets of BCPs are obtained by topological analysis of the theoretical $\rho(\mathbf{r})$ function calculated by PBE0-D3/POB-TZVP method for optimized crystal structures.

d_{12} is the distance between the atoms;
$\rho(r)$, $\nabla^2\rho(\mathbf{r})$ and ε are the value of electron density, laplassian of electron density and ellipticity in the BCP
E_{EML} is the interaction energy estimated by Espinosa–Molins–Lecomte correlation
sym. op. is the symmetry operation that generates Atom 2.

Table S1. Bond critical points corresponding to intramolecular interactions in form **I**.

#	Atom 1	Atom 2	d_{12}, Å	$\rho(\mathbf{r})$, e Å^{-3}	$\nabla^2\rho(\mathbf{r})$, e Å^{-5}	ε
1	O1	N1	1.273	2.73	-10.48	0.10
2	C2	N1	1.414	1.883	-16.62	0.25
3	H3N	O1	1.802	0.266	3.420	0.02
4	N3	C7	1.423	1.834	-17.57	0.05
5	C7	C8	1.386	2.153	-22.83	0.22
6	N1	O2	1.254	2.848	-11.72	0.09
7	N2	O3	1.259	2.815	-11.22	0.09
8	O4	N2	1.260	2.816	-11.26	0.10
9	C4	N2	1.426	1.848	-16.72	0.18
10	C5	C4	1.405	2.081	-21.99	0.16
11	C12	H6	2.445	0.094	1.200	3.20
12	C11	C12	1.380	2.159	-22.77	0.19
13	C4	C3	1.370	2.219	-23.96	0.23
14	C2	C3	1.388	2.142	-22.62	0.21
15	C1	C2	1.429	1.999	-20.60	0.20
16	N3	H3N	1.013	2.255	-45.70	0.03
17	N3	C1	1.335	2.277	-26.22	0.15
18	C6	C1	1.421	2.023	-21.05	0.15
19	C12	C7	1.383	2.168	-23.02	0.23
20	C6	C5	1.355	2.251	-24.05	0.24
21	C3	H3	1.079	1.966	-25.90	0.00
22	C5	H5	1.081	1.956	-25.56	0.00
23	C6	H6	1.080	1.951	-25.07	0.02
24	C9	C8	1.377	2.169	-22.87	0.20
25	C8	H8	1.083	1.930	-24.55	0.01
26	C10	C9	1.390	2.132	-22.31	0.19
27	C9	H9	1.085	1.919	-24.18	0.01
28	C13	C10	1.493	1.761	-16.73	0.03
29	C10	C11	1.387	2.145	-22.47	0.20
30	C11	H11A	1.084	1.919	-24.17	0.01
31	C12	H12	1.081	1.934	-24.57	0.01
32	C13	H13C	1.089	1.878	-22.85	0.01
33	C13	H13A	1.090	1.874	-22.77	0.01
34	C13	H13B	1.093	1.861	-22.51	0.01

Table S2. Bond critical points corresponding to intermolecular interactions in form **I**.

#	Atom 1	Atom 2	d_{12}, Å	$\rho(\mathbf{r})$, e Å^{-3}	$\nabla^2\rho(\mathbf{r})$, e Å^{-5}	ε	E_{EML}	sym.op. for atom 2
1	O2	H9A	3.013	0.02	0.28	0.21	0.47	-x,-y+1,z+1
2	O1	O1	2.892	0.044	0.87	0.47	1.45	-x,-y+1,z
3	O1	H8A	2.402	0.068	0.88	0.04	1.66	-x,-y+1,z+1
4	H3N	O1	2.565	0.034	0.54	1.86	0.86	-x,-y+1,z
5	O2	C3	3.294	0.033	0.50	1.85	0.78	x,y,z+1
6	O2	H13C	2.604	0.048	0.84	0.51	1.58	x-1,y,z+1
7	O2	H13B	2.853	0.027	0.38	0.18	0.65	x-1,y,z
8	O1	H8A	3.048	0.022	0.32	0.30	0.47	-x,-y+1,z
9	C4	C3	3.306	0.040	0.55	1.83	0.90	x,y,z-1
10	O3	H5A	2.643	0.038	0.52	0.04	0.95	x-1/2,-y+1/2,-z+2
11	O4	H12A	2.425	0.066	0.92	0.06	1.80	x-1/2,-y+1/2,-z+1
12	O3	H13A	2.993	0.021	0.25	2.07	0.46	x-1,y,z
13	O4	H6A	2.770	0.032	0.38	0.12	0.70	x-1/2,-y+1/2,-z+2
14	O3	C6	3.673	0.013	0.21	0.66	0.25	x-1/2,-y+1/2,-z+1
15	C4	O4	3.283	0.034	0.49	0.70	0.76	x,y,z+1
16	H3A	H13A	2.308	0.034	0.39	0.12	0.77	x-1,y,z
17	C11	O4	3.233	0.031	0.50	1.48	0.79	x+1/2,-y+1/2,-z+2
18	C6	C1	3.329	0.037	0.55	3.42	0.82	x,y,z-1
19	C8	C7	3.314	0.041	0.61	4.47	0.94	x,y,z-1
20	C13	H13C	2.735	0.046	0.54	0.95	1.16	x,y,z+1
21	H12A	H6A	2.275	0.037	0.42	0.15	0.87	x,y,z+1
22	C10	C11	3.280	0.043	0.62	2.40	1.00	x,y,z-1
23	H13B	H9A	2.316	0.043	0.50	0.35	1.04	-x-1,-y+1,z
24	H13C	C10	2.796	0.043	0.56	6.00	1.14	x,y,z-1

Table S3. Bond critical points corresponding to intramolecular interactions in form **II**.

#	Atom 1	Atom 2	d_{12}, Å	ρ(r), e Å^{-3}	$\nabla^2\rho(\mathbf{r})$, e Å^{-5}	ε
1	O1	N1	1.270	2.750	-10.84	0.10
2	O2	N1	1.250	2.878	-12.14	0.09
3	O3	N2	1.261	2.800	-11.11	0.09
4	O4	N2	1.261	2.806	-11.35	0.09
5	N1	C2	1.421	1.870	-16.84	0.23
6	N2	C4	1.417	1.875	-16.68	0.20
7	N3	C1	1.337	2.259	-25.87	0.15
8	N3	C7	1.420	1.850	-17.9	0.06
9	N3	H3N	1.016	2.248	-45.69	0.03
10	C2	C3	1.382	2.166	-23.03	0.21
11	C4	C5	1.403	2.089	-22.13	0.16
12	C3	C4	1.372	2.207	-23.82	0.22
13	C1	C6	1.419	2.035	-21.26	0.15
14	C7	C8	1.385	2.158	-22.95	0.22
15	C2	C1	1.429	2.000	-20.64	0.20
16	C6	C5	1.355	2.257	-24.19	0.24
17	C6	H6	1.080	1.955	-25.09	0.01
18	C3	H3	1.080	1.963	-25.83	0.00
19	C5	H5	1.079	1.957	-25.5	0.00
20	C7	C12	1.390	2.134	-22.47	0.22
21	C8	C9	1.383	2.150	-22.58	0.19
22	C11	C12	1.379	2.157	-22.59	0.20
23	C8	H8	1.083	1.930	-24.55	0.01
24	C9	H9	1.083	1.926	-24.31	0.01
25	C10	C9	1.390	2.135	-22.29	0.19
26	C13	C10	1.494	1.754	-16.61	0.03
27	C11	C10	1.39	2.129	-22.21	0.19
28	C11	H11	1.085	1.917	-24.1	0.01
29	C12	H12	1.083	1.931	-24.56	0.01
30	C13	H13A	1.089	1.889	-23.17	0.01
31	C13	H13B	1.091	1.862	-22.48	0.01
32	C13	H13C	1.090	1.872	-22.71	0.01
33	O1	H3N	1.826	0.252	3.290	0.02
34	C12	H6	2.478	0.093	1.200	1.58

Table TS3 (continued)

#	Atom 1	Atom 2	d_{12}, Å	ρ(r), e Å^{-3}	$\nabla^2\rho(\mathbf{r})$, e Å^{-5}	ε
35	O1'	N1'	1.270	2.745	-10.67	0.10
36	O2'	N1'	1.252	2.866	-11.98	0.09
37	O3'	N2'	1.261	2.805	-11.20	0.09
38	O4'	N2'	1.260	2.808	-11.26	0.09
39	N1'	C2'	1.419	1.875	-16.87	0.23
40	N2'	C4'	1.420	1.869	-16.79	0.19
41	N3'	C1'	1.338	2.256	-25.84	0.14
42	N3'	C7'	1.417	1.861	-18.15	0.06
43	N3'	H3N'	1.014	2.260	-45.67	0.03
44	C2'	C3'	1.383	2.162	-22.97	0.21
45	C3'	C4'	1.372	2.210	-23.84	0.22
46	C4'	C5'	1.402	2.090	-22.14	0.16
47	C6'	C1'	1.418	2.037	-21.27	0.15
48	C8'	C7'	1.389	2.147	-22.78	0.22
49	C1'	C2'	1.428	2.006	-20.74	0.20
50	C5'	C6'	1.355	2.257	-24.22	0.24
51	C3'	H3'	1.079	1.964	-25.80	0.00
52	C5'	H5'	1.081	1.954	-25.39	0.00
53	C6'	H6'	1.079	1.957	-25.14	0.02
54	C7'	C12'	1.388	2.144	-22.64	0.22
55	C8'	C9'	1.382	2.149	-22.48	0.20
56	C12'	C11'	1.382	2.151	-22.52	0.20
57	C8'	H8'	1.084	1.930	-24.59	0.01
58	C9'	H9'	1.083	1.919	-24.13	0.01
59	C9'	C10'	1.391	2.128	-22.20	0.19
60	C10'	C11'	1.388	2.138	-22.33	0.19
61	C10'	C13'	1.495	1.755	-16.63	0.03
62	C11'	H11'	1.084	1.928	-24.40	0.01
63	C12'	H12'	1.084	1.933	-24.62	0.01
64	C13'	H13D	1.089	1.886	-23.08	0.01
65	C13'	H13E	1.092	1.855	-22.34	0.01
66	C13	H13F'	1.089	1.879	-22.89	0.01
67	O1'	H3N'	1.843	0.244	3.210	0.04
68	H6'	C12'	2.465	0.096	1.240	1.15

Table S4. Bond critical points corresponding to intermolecular interactions in form **II**.

#	Atom 1	Atom 2	d_{12}, Å	$\rho(\mathbf{r})$, e Å^{-3}	$\nabla^2\rho(\mathbf{r})$, e Å^{-5}	ε	E_{EML}	sym. op. for atom 2
1	C2'	C10	3.333	0.041	0.54	1.03	0.87	x-1,y+1,z
2	N1'	C9	3.252	0.038	0.59	0.54	1.03	x-1,y+1,z
3	H8'	O1'	2.720	0.037	0.49	0.78	0.87	-x,-y,-z-1
4	C6'	H13C	2.619	0.059	0.68	0.93	1.53	x+1,y-1,z
5	H3N'	O1'	2.601	0.035	0.53	1.39	0.86	-x,-y,-z-1
6	O1'	H9	2.550	0.043	0.62	0.12	1.13	-x+1,-y-1,-z-1
7	H8'	O2'	2.561	0.049	0.64	0.05	1.17	-x,-y,-z-1
8	H13F	O2'	2.687	0.044	0.75	0.53	1.39	x,y+1,z
9	O2'	C11	3.265	0.038	0.54	1.75	0.87	x,y-1,z
10	O3'	H12'	2.471	0.059	0.75	0.01	1.42	-x,-y,-z
11	O3'	H5	2.554	0.043	0.71	0.25	1.28	x-1,y+1,z
12	O3'	H6	2.575	0.050	0.71	0.16	1.36	x-1,y+1,z
13	O3'	O3	3.488	0.016	0.23	0.02	0.33	-x,-y,-z
14	N2'	C6'	3.382	0.036	0.60	7.55	0.97	-x,-y,-z
15	O3'	O3	3.850	0.007	0.10	0.65	0.14	-x+1,-y,-z
16	O4'	H11	2.470	0.052	0.73	0.03	1.37	-x,-y-1,-z
17	O4'	H13C	3.057	0.019	0.32	0.90	0.47	-x,-y-1,-z
18	C5'	O4'	3.852	0.008	0.14	0.53	0.15	-x-1,-y,-z
19	O1'	H13B	2.821	0.033	0.44	0.12	0.80	x,y-1,z
20	N3'	H13B	2.895	0.030	0.36	0.21	0.66	x,y-1,z
21	O1'	O1'	2.924	0.046	0.85	0.55	1.43	-x,-y,-z-1
22	H3'	H6	2.339	0.034	0.40	0.19	0.80	x-1,y+1,z
23	C3'	C11	3.498	0.026	0.45	1.55	0.59	x-1,y+1,z
24	H5'	O3	2.716	0.033	0.57	1.39	0.98	x-1,y,z
25	H6'	O3	2.350	0.075	1.09	0.07	2.17	x-1,y,z
26	C8'	H8	2.796	0.039	0.42	0.20	0.86	-x+1,-y-1,-z-1
27	C12'	O2	3.138	0.045	0.61	0.62	1.11	x,y,z
28	H8'	H13A	2.893	0.012	0.18	0.36	0.26	x-1,y+1,z
29	C9'	C2	3.254	0.049	0.61	2.13	1.10	x-1,y,z
30	C13'	H9'	2.851	0.038	0.49	1.60	0.98	-x,-y-1,-z-1
31	H9'	H9'	2.312	0.040	0.46	0.14	0.95	-x,-y-1,-z-1
32	C13'	C6	3.300	0.043	0.61	5.02	1.19	x-1,y,z
33	H11'	O4	2.307	0.069	1.05	0.04	1.97	-x+1,-y-1,-z
34	C11'	C4	3.415	0.032	0.49	0.93	0.70	x-1,y,z
35	O4	C6	3.242	0.041	0.63	2.98	1.06	-x+1,-y-1,-z
36	H13E	N3	2.784	0.039	0.50	0.26	0.94	x,y,z
37	H13F	N3	2.749	0.048	0.63	1.91	1.23	x-1,y,z
38	H13D	O4	2.756	0.031	0.41	0.12	0.75	-x+1,-y-1,-z
39	O1	O1	2.743	0.062	1.25	0.53	2.33	-x+1,-y-1,-z-1
40	H3N	O1	2.387	0.050	0.83	0.50	1.31	-x+1,-y-1,-z-1
41	H8	O1	2.792	0.037	0.50	0.14	0.87	-x+1,-y-1,-z-1
42	O2	C13	3.049	0.041	0.75	0.93	1.35	x,y-1,z
43	H8	O2	2.877	0.031	0.44	0.17	0.73	-x+1,-y-1,-z-1
44	H12	O3	2.503	0.056	0.72	0.04	1.37	-x+1,-y-1,-z
45	H12	O4	2.697	0.038	0.50	2.89	0.93	-x+1,-y-1,-z
46	O4	H5	3.382	0.009	0.14	0.29	0.17	-x+2,-y-1,-z
47	H13A	H9	2.571	0.032	0.45	2.06	0.83	-x+1,-y-2,-z-1

5. Powder diffraction pattern of form I.

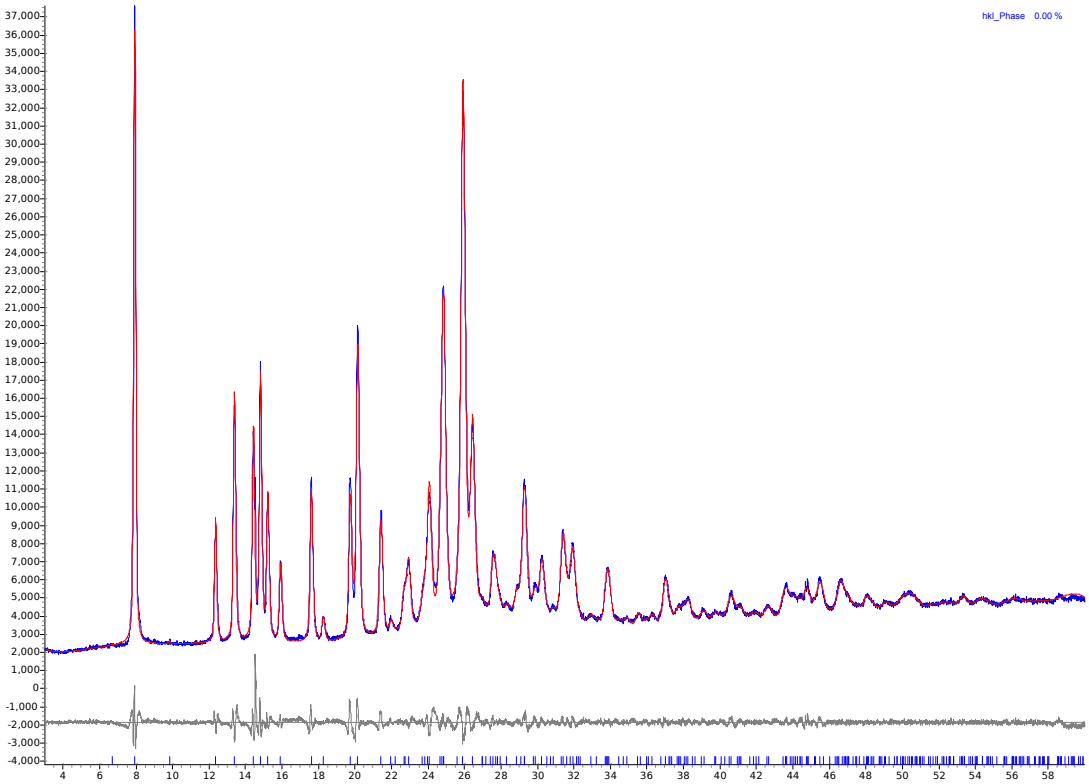

Figure. S3. Observed (blue line) and calculated (red line, Pawley fit, Rwp=0.0354) powder diffraction patterns for the crystal structure of form **I**.

The refined unit cell parameters (sp. gr. $P2_12_12$):
a = 12.270(2), b = 26.473(4), c = 3.9189(5) Å, V = 1271.3(4) Å^3, d_{calc} = 1.428 g cm^{-3}.

X-ray powder diffraction study of the form **I** was performed on a Bruker AXS D8 diffractometer equipped with a primary monochromator (CuKα_1, λ =1.54056 Å) and a LynxEye position sensitive detector. The sample was deposited on a zero-background silicon plate and were rotated with a speed of 60 deg·min^{-1}. Data collections was performed in the reflection mode at ambient temperature (ca. 298 K) with a step size of 0.01° for the 2θ range of 5–60°. The unit cell parameters and phase purity of the bulk sample were evaluated by a Pawley fit starting from the single-crystal unit cell parameters. The calculations were performed with the Bruker TOPAS 5.0 software [A. A. Coelho, *J. Appl. Crystallogr.*, 2018, **51**, 210–218; doi: 10.1107/S1600576718000183].

6. Differential scanning calorimetry for form I

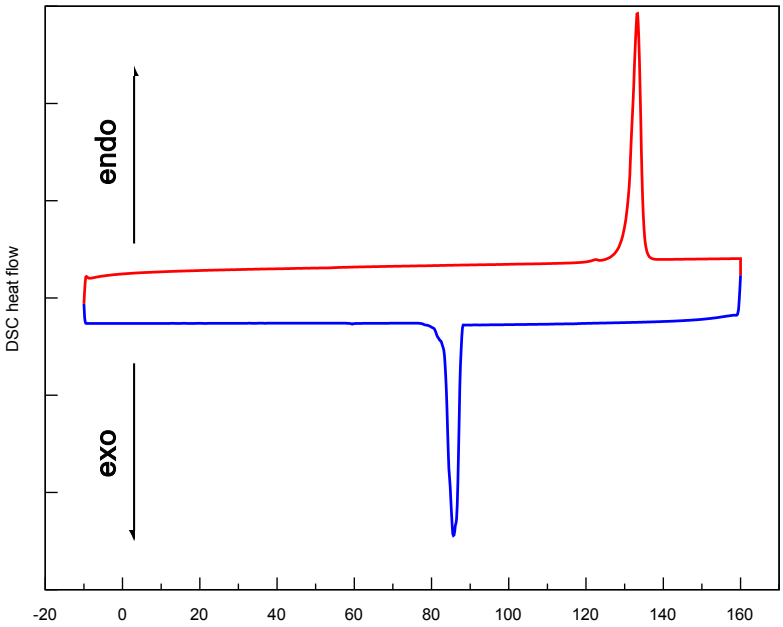

Figure. S4. DSC curves for the powder sample of form **I** upon heating (upper red curve) and cooling (lower blue curve) within the temperatures range −10 – 170 °C.

The calorimetric studies were performed on a Mettler-822e differential scanning calorimeter. The weight of the sample was 2.7 mg, the heating/cooling rate was 10 °C min^{-1}.