Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary information

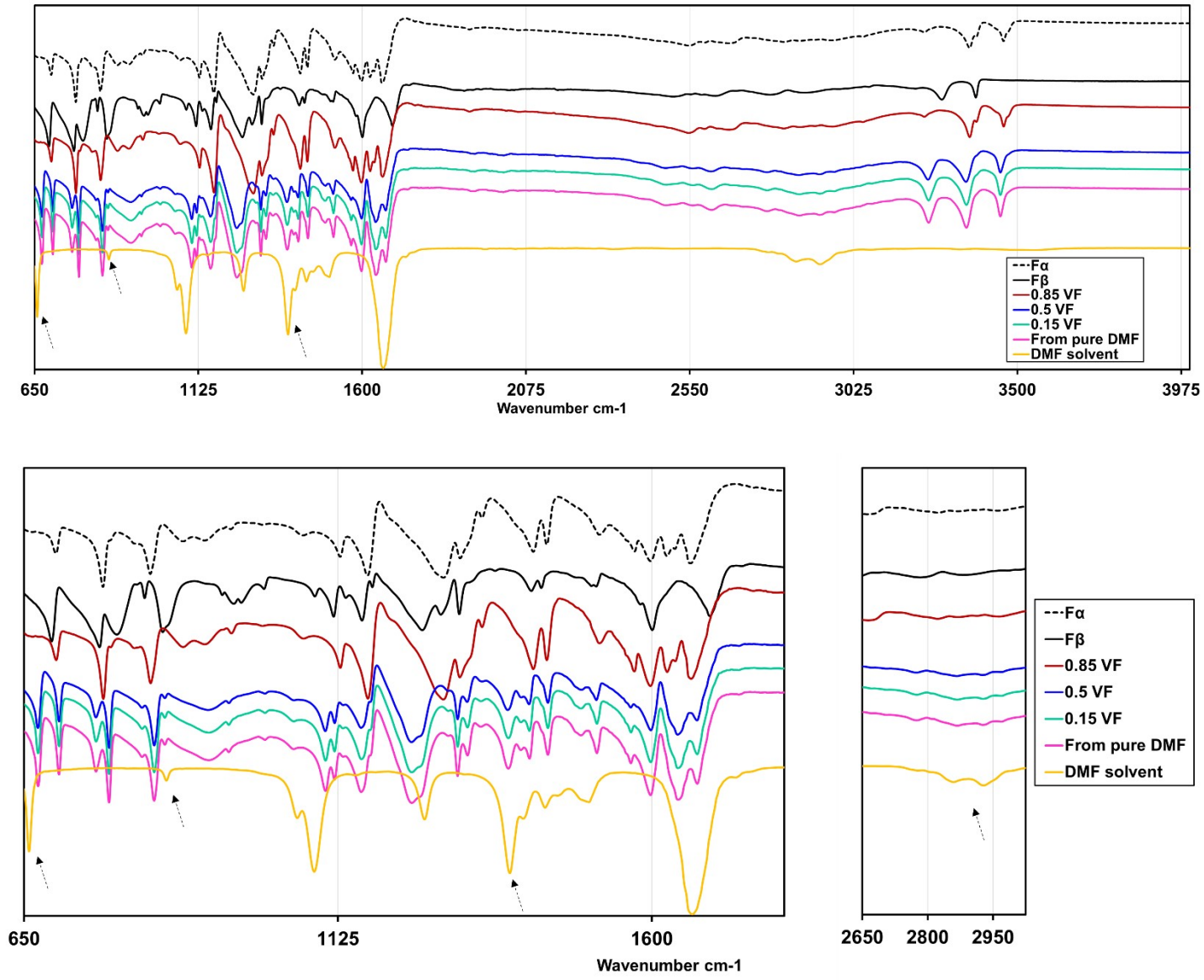

Figure S1. (Top) Full ATR-FTIR plots for experiments with DMF-water system and standard curves for Fα and Fβ. Results at 0.85 VF yields Fα, experiments with VF of 0.5 and higher yield the new form. (Bottom) Region between 650 – 1800 cm^{-1} and 2650 – 3025 cm^{-1}.

Single crystal XRD measurement

X-ray intensity data were collected at 293(2) K on an Agilent SuperNova diffractometer with Eos CCD detector using Mo-Kα radiation (λ = 0.71073 Å). The images were interpreted and integrated with CrysAlisPRO [1] and the implemented absorption correction was applied. The structures were solved using Olex2 [2] with the ShelXT [3] structure solution program using Intrinsic Phasing and refined with the ShelXL [4] refinement package using full-matrix least-squares minimization on F^2. The amine and carboxylic acid hydrogen atoms H1A, H1B and H2 were located in a difference-Fourier map and refined freely. Non-hydrogen atoms were refined anisotropically and hydrogen atoms bound to carbon in the riding mode with isotropic temperature factors fixed at 1.2 times U_{eq} of the parent atoms (1.5 times U_{eq} for methyl groups). Crystal data, data collection and structure refinement details are summarized in Table S1. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre and allocated the deposition number CCDC 2279352. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1 Crystal data and structure refinement for p-ABA/DMF solvate.

Empirical formula	$C_{10}H_{14}N_2O_3$
Formula weight	210.23
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.1603(7)
b/Å	11.1181(8)
c/Å	11.9004(9)
α/°	90
β/°	110.772(9)
γ/°	90
Volume/Å^3	1133.22(16)
Z	4
ρ_{calc}g/cm^3	1.232
μ/mm^{-1}	0.092
F(000)	448.0
Crystal size/mm^3	0.5 × 0.45 × 0.25
Radiation	Mo Kα (λ = 0.71073 Å)
2Θ range for data collection/°	4.866 to 52.732
Index ranges	$-11 \le h \le 11$, $-13 \le k \le 13$, $-14 \le l \le 14$
Reflections collected	11747
Independent reflections	2308 [R_{int} = 0.0218, R_{sigma} = 0.0170]
Data/restraints/parameters	2308/0/151
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0510, wR_2 = 0.1402
Final R indexes [all data]	R_1 = 0.0680, wR_2 = 0.1563
Largest diff. peak/hole / e Å^{-3}	0.21/-0.16

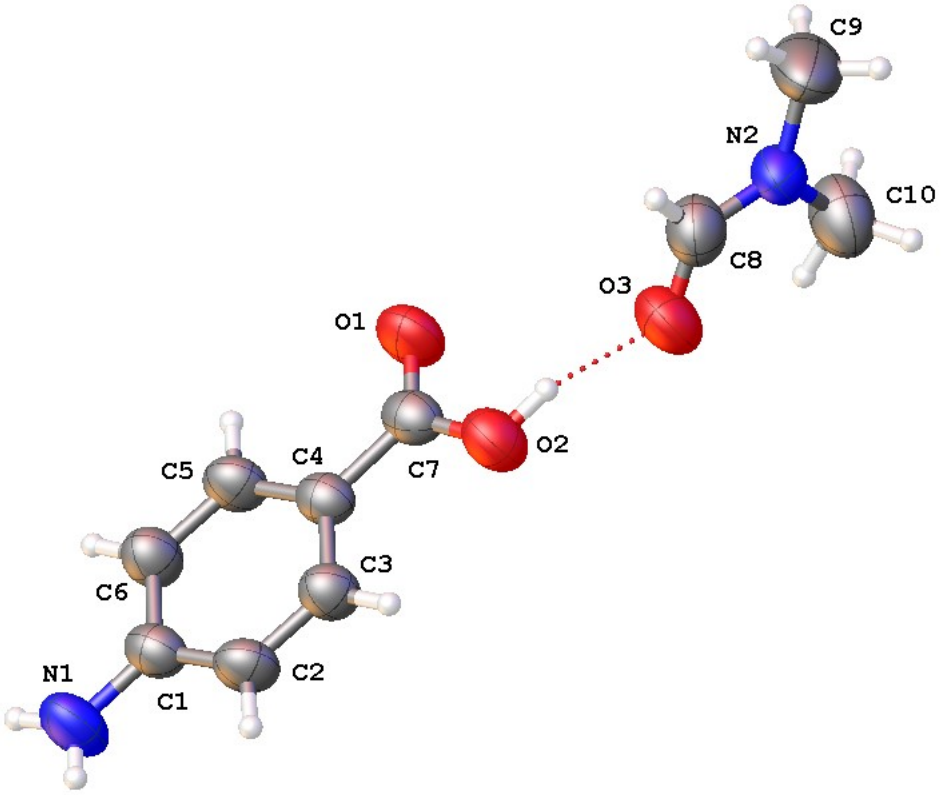

Figure S2. Molecular structure of the *p*-ABA/DMF solvate showing atom labelling and thermal ellipsoids drawn at 30% probability level.

References

1. CrysAlis PRO (2012). Agilent Technologies UK Ltd, Yarnton, Oxfordshire, England.
2. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, J. Appl. Cryst., 2009, **42**, 339-341.
3. G.M. Sheldrick, Acta. Cryst., 2015, A71, 3-8.
4. G.M. Sheldrick, Acta. Cryst., 2015, C71, 3-8.