Electronic Supplementary Information (ESI) for:

Some thoughts about the single crystal growth of small molecules

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Experimental methods

Most chemicals were purchased from Sigma-Aldrich. Tetrahydropyran and 1,2-difluorobenzene were from ABCR. Tablet tubes (40 mm x 12.75 mm) were from Müller-Krempel (Switzerland). Glass scintillation vials (20 ml, 61 mm x 28 mm) were from Wheaton.

Single crystal data were collected at 183(2) K on an Oxford Diffraction Xcalibur system with a Ruby detector using Mo K_α radiation (λ = 0.7107 Å) that was graphite-monochromated. A suitable crystal was covered with oil (Infineum V8512, formerly known as Paratone N), mounted on top of a glass fibre and immediately transferred to the diffractometer. The program suite CrysAlis^{Pro} was used for data collection, multi-scan absorption correction and data reduction.[1] The structures were solved with direct methods using SIR97[2] and refined by full-matrix least-squares methods on F^2 with SHELXL-97.[3] The final structures were checked for higher symmetry with help of the program Platon.[4] CCDC 849680 and 800843 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Powder X-ray diffraction (XRD) was performed at room temperature on a STOE STADI P diffractometer in transmission mode (flat sample holders, Ge monochromator and Cu $K_{\alpha1}$ radiation).

Table S1: Crystallographic data for 1 and 2.

Compound	**1**	**2**
Empirical formula	$C_{24}H_{22}N_4O_4$	$C_{12}H_{11}NO_2$
Space group	$P2_1/c$	P-1
a [Å]	9.3329(2)	7.5975(5)
b [Å]	12.7049(3)	12.2026(7)
c [Å]	9.1195(2)	12.8137(8)
α [°]	90	61.607(6)
β [°]	98.085(2)	77.247(5)
γ [°]	90	78.353(5)
Volume [$Å^3$]	1070.59(4)	1012.74(11)
Z	2	4
Crystal size [mm^3]	0.50 x 0.27 x 0.11	0.21 x 0.13 x 0.08
Independent reflections	3660 [R(int) = 0.0209]	5457 [R(int) = 0.0402]
Reflections observed (>2sigma(I))	3116	2329
Completeness to theta	99.9 % to 30.44°	99.9 % to 29.13°
Max. and min. transmission	0.9898 and 0.7360	0.9928 and 0.8558
Data / restraints / parameters	3660 / 0 / 146	5457 / 0 / 273
Goodness-of-fit on F^2	1.032	0.810
Final R indices (I>2sigma(I))	R1 = 0.0464, wR2 = 0.1216	R1 = 0.0479, wR2 = 0.0782
Largest diff. peak and hole [$e.Å^{-3}$]	0.405 and -0.223	0.163 and -0.268

Figure S1:

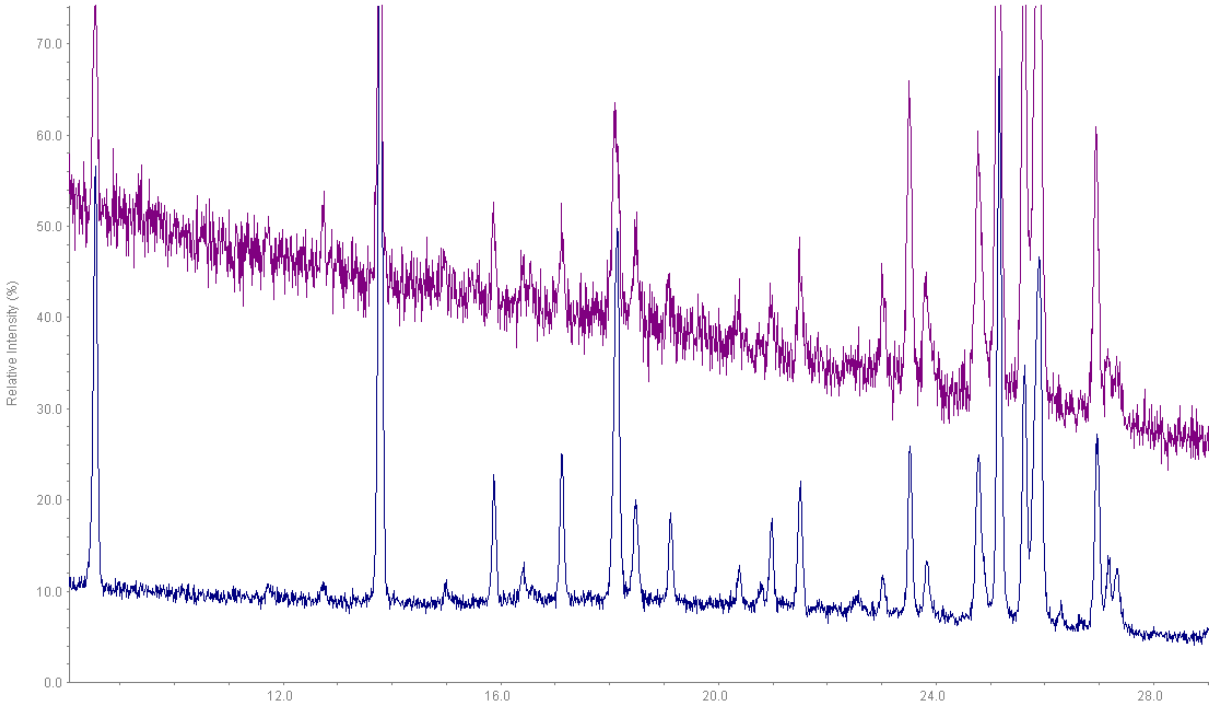

Fig. S1: Powder diffractograms of **2** grown from either chloroform against cyclohexane (top) or trichloroethylene against heptane (bottom).

1. Oxford Diffraction Ltd., *CrysAlis^{Pro} Software system*, (2007), Oxford, UK.
2. A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori and R. Spagna, *J. Appl. Cryst.*, 1999, **32**, 115-119.
3. G. M. Sheldrick, *Acta Crystallogr D*, 2008, **A64**, 112-122.
4. A. L. Spek, *J. Appl. Cryst.*, 2003, **36**, 7-13.