Supporting information for

Influence of the solvent of crystallization on the orientational disorder of (*trans*)-4-chloro-4′-nitrostilbene

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Table S1: Cell parameters determined for $P2_1$ model.

sample	ClBz II	NO_2Bz II	EtOH	ClBz I	ClBz III	ClBz IV	ClTol	Tol I	Tol II	NO_2Bz I
radiation	synchrotron, $\lambda = 0.7100(5)$ Å			sealed tube, Mo Kα, $\lambda = 0.71073$ Å						
a (Å)	3.91412(16)	3.91649(10)	3.91514(5)	3.9200(3)	3.9164(2)	3.9100(2)	3.9182(2)	3.9236(3)	3.9239(2)	3.9220(2)
b (Å)	12.9559(6)	12.9357(3)	12.96036(16)	12.9790(10)	12.9581(6)	12.9349(7)	12.9555(8)	12.9740(8)	12.9733(6)	12.9245(7)
c (Å)	12.2307(6)	12.3004(3)	12.22634(16)	12.2368(9)	12.2370(5)	12.2210(6)	12.2381(7)	12.2406(7)	12.2398(6)	12.3038(7)
β (°)	93.221(4)	92.999(2)	93.1916(12)	93.153(3)	93.238(2)	93.352(2)	93.254(3)	93.175(3)	93.192(2)	92.957(2)
V (Å^3)	619.25(8)	622.32(3)	619.422(14)	621.63(12)	620.03(5)	617.03(12)	620.24(10)	622.15(10)	622.11(8)	622.85(9)
ρ (g cm^{-3})	1.39	1.39	1.39	1.39	1.39	1.40	1.390	1.39	1.39	1.39

sample	Me_2CO	EtOAc	MeCN I	MeCN II	DMF I	DMF II	DMSO I[a]	DMSO II[a]	MeOH	statistical analysis	
radiation	sealed tube, Mo Kα, $\lambda = 0.71073$ Å									present data	<bz>[b]
a (Å	3.9118(2)	3.9227(2)	3.9216(3)	3.9221(4)	3.9208(2)	3.9220(2)	3.9192(1)	3.9173(1)	3.9239(3)	3.919(4)	3.921(4)
b (Å)	12.9470(5)	12.9764(7)	12.9663(10)	12.9733(12)	12.9696(7)	12.9786(5)	12.9630(4)	12.9563(3)	12.9707(9)	12.961(15)	12.961(12)
c (Å)	12.2260(4)	12.2535(6)	12.2348(9)	12.2509(12)	12.2508(7)	12.2507(6)	12.2399(4)	12.2343(3)	12.2375(8)	12.245(20)	12.207(17)
β (°)	93.191(2)	93.200(2)	93.153(3)	93.149(3)	93.138(2)	93.128(2)	93.188(2)	93.151(1)	93.236(3)	93.172(81)	93.248(15)
V (Å^3)	618.24(6)	622.76(6)	621.18(8)	622.42(11)	622.03(9)	622.65(7)	620.89(5)	619.99(4)	621.84(8)	621.0 (1.5)	619.2 (2.1)
ρ (g cm^{-3})	1.40	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.389(3)	1.393(5)

[a] DMSO I and DMSO II refer to the same crystal.

[b] Analysis of 9 diffraction experiments with 7 different samples grown from benzene, as reported in Reference 3.

Table S2: *R*-ratio test of significance between the $P2_1$ model and the pseudo $P2_1/c$ model.

Sample	ClBz I	ClBz II	ClBz III	ClBz IV	ClTol	Tol I	Tol II	NO_2Bz I	NO_2Bz II	Me_2CO
Test 1 $= \frac{R1(I>2\sigma(I))(P2_1/c)}{R1(I>2\sigma(I))(P2_1)}$	1.220	1.000	1.167	1.174	1.087	1.132	1.204	1.019	1.018	1.023
Test 2 $= \frac{R1(\text{all reflections})(P2_1/c)}{R1(\text{all reflections})(P2_1)}$	1.098	1.000	1.089	1.082	1.041	1.058	1.102	1.009	1.000	1.031
Test 3 $= \frac{wR2(P2_1/c)}{wR2(P2_1)}$	1.218	1.012	1.211	1.162	1.131	1.143	1.227	1.011	1.015	1.075
$R_{p,n-p}$ at $p=0.005$	1.029	1.019	1.022	1.023	1.026	1.025	1.021	1.027	1.018	1.024
$R_{p,n-p}$ at $p=0.05$	1.007	1.004	1.005	1.006	1.006	1.006	1.005	1.007	1.004	1.006

Sample	EtOAc	MeCN I	MeCN II	DMF I	DMF II	DMSO I[a]	DMSO II[a]	EtOH	MeOH
Test 1 $= \frac{R1(I>2\sigma(I))(P2_1/c)}{R1(I>2\sigma(I))(P2_1)}$	1.194	1.000	1.000	1.000	1.048	1.024	1.047	1.091	1.200
Test 2 $= \frac{R1(\text{all reflections})(P2_1/c)}{R1(\text{all reflections})(P2_1)}$	1.105	1.000	1.000	1.009	1.014	1.017	1.016	1.098	1.090
Test 3 $= \frac{wR2(P2_1/c)}{wR2(P2_1)}$	1.248	1.000	1.000	1.017	1.053	1.043	1.067	1.195	1.245
$R_{p,n-p}$ at $p=0.005$	1.026	1.031	1.034	1.026	1.026	1.022	1.016	1.015	1.023
$R_{p,n-p}$ at $p=0.05$	1.006	1.007	1.008	1.006	1.006	1.005	1.004	1.004	1.006

$p=1$, n = number of unique reflections with $I>2\sigma(I)$ (see Table 1).

[a] DMSO I and DMSO II refer to the same crystal.

Table S3: Presence of superstructure reflections $k'_o l'_o$.

solvent	n[a]	$\langle I/\sigma \rangle$	$n(I > 2\sigma(I))$	%[b]	expression
Tol I	594	1.56	195	32.83	++
Tol II	717	3.20	395	55.09	++
EtOAc	634	0.67	103	16.25	+
Me_2CO	804	0.74	160	19.90	+
DMSO II	4411	0.13	234	5.30	+
$\langle$Bz$\rangle$[c]	3904	5.01	2061	52.79	++

[a] From Table 2.
[b] Percentage of n with $I > 2\sigma(I)$ compared to n.
[c] See reference 3.

Table S4: Correlation coefficients between the S.O.F. p's in the $A1$ model.

sample correlation	Me_2CO	DMSO II	EtOAc	Tol I	Tol II
p_C, p_A	−0.955	−0.641	−0.733	0.952	−0.639
p_D, p_A	−0.953	−0.638	−0.678	0.953	−0.614
p_A, p_A	−0.973	−0.997	−0.651	−0.876	−0.900
p_C, p_A	0.949	0.637	0.526	−0.963	0.443
p_D, p_A	0.946	0.634	0.486	−0.964	0.426
p_D, p_C	−0.880	−0.273	−0.132	−0.993	0.196

Table S5: Sums and differences of S.O.F.s with s.u.'s in $A1$ model.

solvent	$p_A + p_B$	$p_A - p_B$	$p_C + p_D$	$p_C - p_D$
Tol I	0.879(10)	0.247(39)	0.698(9)	−0.062(146)
Tol II	0.841(10)	0.043(45)	0.738(9)	0.288(8)
EtOAc	0.838(8)	0.068(18)	0.651(8)	0.149(9)
Me_2CO	0.988(6)	0.042(50)	0.818(5)	0.102(21)
DMSO II	0.980(4)	0.002(106)	0.848(4)	0.038(5)
$\langle$Bz$\rangle$[a]	0.926(20)	0.113(33)	0.822(20)	0.391(63)

[a] See reference 3.

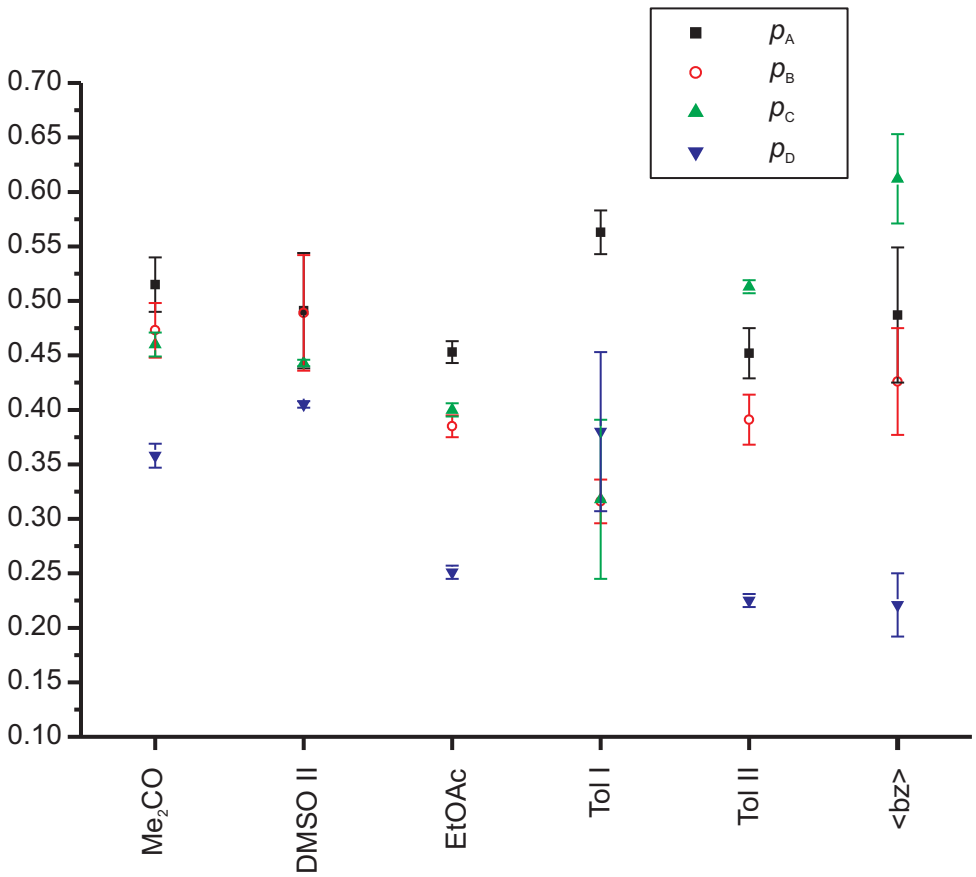

Figure S1: S.O.F. populations p_A, p_B, p_C, p_D for different specimens. The data for $\langle bz \rangle$ represent the average and s.u.s for 9 separate experiments (see reference 3).

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