Supporting information: Carbamazepine crystal precipitated from microemulsion containing 40 wt% aqueous phase.

Table 1. Crystal data and structure refinement for crystal obtained from microemulsion containing 40 wt% aqueous phase.

Identification code	anna31m	
Empirical formula	C15 H16 N2 O3	
Formula weight	272.30	
Temperature	295(1)K	
Wavelength	0.71073Å	
Crystal system	Orthorhombic	
Space group	Cmca	
Unit cell dimensions	a = 19.779(2)Å	α=90°.
	b = 4.9369(4)Å	β=90°.
	c = 28.714(3)Å	γ=90°.
Volume	2803.8(4) $Å^3$	
Z	8	
Density (calculated)	1.290 g/cm^3	
Absorption coefficient	0.091 mm^{-1}	
F(000)	1152	
Crystal size	0.24 × 0.16 × 0.13 mm^3	
Theta range for data collection	2.84 to 28.01°	
Index ranges	-25≤h≤25, -6≤k≤6, -36≤l≤36	
Reflections collected	15488	
Independent reflections	1732 [R(int) = 0.0381]	
Completeness to theta = 28.01°	98.7%	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	1732/0/102	
Goodness-of-fit on F^2	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0510, wR2 = 0.1464	
R indices (all data)	R1 = 0.0670, wR2 = 0.1548	
Largest diff. peak and hole	0.314 and -0.193 e x $Å^{-3}$	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for crystal obtained from microemulsion containing 40 wt% aqueous phase. U(eq) is defined as one-third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9386(1)	3357(3)	6341(1)	35(1)
C(2)	8961(1)	5373(3)	6171(1)	43(1)
C(3)	8358(1)	5924(3)	6393(1)	47(1)
C(4)	8179(1)	4503(3)	6787(1)	46(1)
C(5)	8602(1)	2528(3)	6959(1)	43(1)
C(6)	9219(1)	1926(3)	6746(1)	35(1)
C(7)	9663(1)	-116(3)	6953(1)	39(1)
C(8)	10000	1594(4)	5666(1)	38(1)
N(1)	10000	2733(4)	6103(1)	37(1)
N(2)	9433(1)	1056(3)	5471(1)	50(1)
O(1)	9433(1)	1056(3)	5471(1)	50(1)
O(1W)	7920(1)	581(3)	5484(1)	79(1)

Table 3. Bond lengths (Å) and angles (°) for crystal obtained from microemulsion containing 40 wt% aqueous phase.

Bond lengths (Å)	
C(1)-C(2)	1.392(2)
C(1)-C(6)	1.398(2)
C(1)-N(1)	1.4283(16)
C(2)-C(3)	1.378(2)
C(2)-H(2)	0.9300
C(3)-C(4)	1.378(2)
C(3)-H(3)	0.9300
C(4)-C(5)	1.377(2)
C(4)-H(4)	0.9300
C(5)-C(6)	1.3970(19)
C(5)-H(5)	0.9300
C(6)-C(7)	1.462(2)
C(7)-C(7)#1	1.335(3)
C(7)-H(7)	0.9300
C(8)-N(2)	1.2821(16)
C(8)-O(1)#1	1.2821(16)
C(8)-N(2)#1	1.2821(16)
C(8)-N(1)	1.375(2)
N(1)-C(1)#1	1.4283(16)
N(2)-H(1N2)	0.93(3)
N(2)-H(2N2)	0.84(3)
O(1W)-H(2N2)	2.29(3)

Angles (°)	
C(2)-C(1)-C(6)	120.74(14)
C(2)-C(1)-N(1)	119.96(15)
C(6)-C(1)-N(1)	119.30(14)
C(3)-C(2)-C(1)	120.08(15)
C(3)-C(2)-H(2)	120.0
C(1)-C(2)-H(2)	120.0

C(4)-C(3)-C(2)	120.08(15)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(5)-C(4)-C(3)	119.89(15)
C(5)-C(4)-H(4)	120.1
C(3)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	121.69(15)
C(4)-C(5)-H(5)	119.2
C(6)-C(5)-H(5)	119.2
C(5)-C(6)-C(1)	117.48(14)
C(5)-C(6)-C(7)	119.50(13)
C(1)-C(6)-C(7)	123.01(13)
C(7)#1-C(7)-C(6)	126.84(8)
C(7)#1-C(7)-H(7)	116.6
C(6)-C(7)-H(7)	116.6
N(2)-C(8)-O(1)#1	122.2(2)
N(2)-C(8)-N(2)#1	122.2(2)
N(2)-C(8)-N(1)	118.89(10)
O(1)#1-C(8)-N(1)	118.89(10)
N(2)#1-C(8)-N(1)	118.89(10)
C(8)-N(1)-C(1)#1	121.70(8)
C(8)-N(1)-C(1)	121.70(8)
C(1)#1-N(1)-C(1)	116.60(16)
C(8)-N(2)-H(1N2)	113.5(19)
C(8)-N(2)-H(2N2)	125(2)
H(1N2)-N(2)-H(2N2)	121(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,z

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for crystal obtained from microemulsion containing 40 wt% aqueous phase. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	36(1)	37(1)	31(1)	-7(1)	-1(1)	-2(1)
C(2)	50(1)	41(1)	36(1)	0(1)	-6(1)	1(1)
C(3)	46(1)	44(1)	51(1)	-9(1)	-9(1)	9(1)
C(4)	37(1)	52(1)	50(1)	-12(1)	1(1)	2(1)
C(5)	41(1)	48(1)	40(1)	-3(1)	4(1)	-7(1)
C(6)	38(1)	35(1)	33(1)	-5(1)	-2(1)	-5(1)
C(7)	46(1)	35(1)	37(1)	2(1)	2(1)	-3(1)
C(8)	48(1)	40(1)	28(1)	-1(1)	0	0
N(1)	39(1)	46(1)	26(1)	-4(1)	0	0
N(2)	45(1)	70(1)	34(1)	-13(1)	-1(1)	-1(1)
O(1)	45(1)	70(1)	34(1)	-13(1)	-1(1)	-1(1)
O(1W)	105(1)	71(1)	62(1)	-1(1)	-7(1)	5(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for crystal obtained from microemulsion containing 40 wt% aqueous phase.

	x	y	z	U(eq)
H(2)	9083	6350	5907	51
H(3)	8072	7257	6276	56
H(4)	7772	4877	6936	56
H(5)	8474	1570	7223	51
H(7)	9452	-1566	7100	47
H(1N2)	9474(16)	470(70)	5165(11)	46(10)
H(2N2)	9049(17)	1360(60)	5588(11)	35(9)

Table 6. Hydrogen bonds for crystal obtained from microemulsion containing 40 wt% aqueous phase (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2N2)...O(1W)	0.84(3)	2.29(3)	3.001(2)	143(3)
N(2)-H(1N2)...N(2)#2	0.93(3)	1.98(3)	2.899(3)	171(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y,z #2 x,-y,-z+1