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Microphase Separation upon Crystallization of Small Amphiphilic Molecules: 'Low' Temperature Form II of Sodium Benzoate (E 211)

T. W. Martin,[a] T. E. Gorelik,*[b] D. Greim,[c] C. Butterhof,[a] U. Kolb,[b] J. Senker,*[c] and J. Breu*[a]

[a] *Department of Inorganic Chemistry I, University of Bayreuth, Universitätsstraße 30, Bayreuth, 95440, Germany. E-mail: josef.breu@uni-bayreuth.de*

[b] *Institute of Physical Chemistry, University of Mainz, Jakob Welder Weg 11, Mainz, 55128, Germany. E-mail: gorelik@uni-mainz.de*

[c] *Department of Inorganic Chemistry III, University of Bayreuth, Universitätsstraße 30, Bayreuth, 95440, Germany. E-mail: juergen.senker@uni-bayreuth.de*

Supporting information

Figures

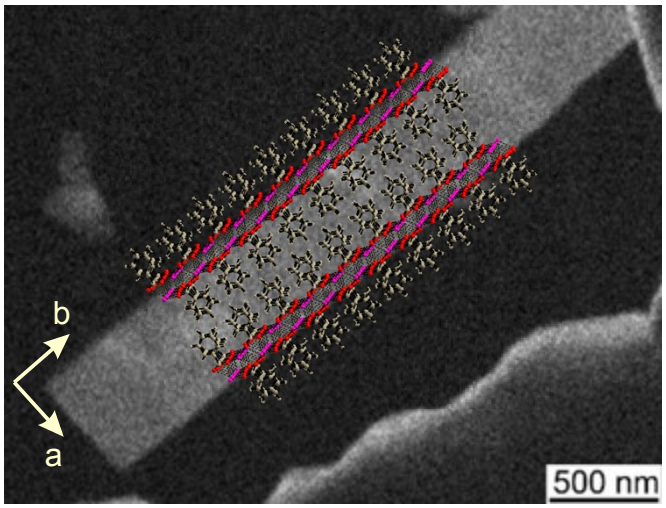

Fig. S1 STEM image of a NaBz form II crystal. All crystals had well-defined faceted form. Unit cell vectors determined from the electron diffraction data allowed to correlate the crystallographic directions and the crystal facets: the rod-like micelles are running along the long direction of the crystals.

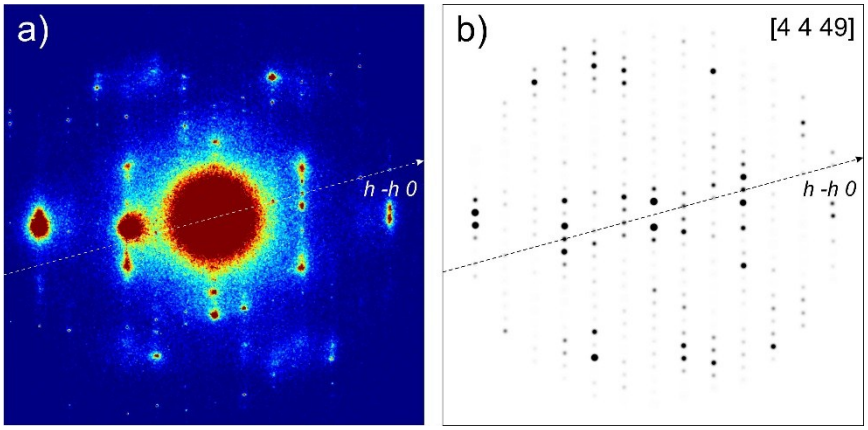

Fig. S2 a) experimental electron diffraction pattern of NaBz form II viewed along the [4 4 49] crystallographic direction, the contrast is enhanced in order to express the diffuse scattering features; b) simulated electron diffraction pattern (eMap, Analitex, Stockholm) of the obtained structure model viewed along the [4 4 49] direction.

Tables

Table S1. Na-O distances in the polyhedra. Corresponding symmetry operations other than (x, y, z) are given in brackets.

	Na1	Na2	Na3	Na4	Na5	Na6
Coordination number	5	6	6	6	6	5
O11 [Å]	2.50(3) (x, 1+y, z)				2.59(3)	2.21(3)
O12 [Å]	2.42(3) (x, 1+y, z)					2.17(2) (x, 1+y, z)
O21 [Å]		2.34(3)			2.34(3)	2.47(3)
O22 [Å]		2.73(3)		2.39(3)	2.33(3) (x, -1+y, z)	
O31 [Å]			2.58(3); 2.43(3) (1-x, 1-y, 1-z)	2.35(3)		
O32 [Å]			2.57(3)	2.35(3) (x, 1+y, z)	2.42(3)	
O41 [Å]			2.37(3) (x, -1+y, z)	2.46(3); 2.45(3) (1-x, 2-y, 1-z)		
O42 [Å]		2.51(3)	2.19(3)	2.42(3)		
O51 [Å]		2.28(3)	2.40(3)		2.68(3)	
O52 [Å]	2.30(3) (x, 1+y, z)	2.31(3) (x, 1+y, z)			2.48(3)	
O61 [Å]	2.38(2)	2.54(3)				2.74(3)
O62 [Å]	2.37(2) (x, 1+y, z)					2.47(2)

Rigid body for crystal structure solution

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load z_matrix {
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Na6  Na1 @  3.8 min 3.25 max 4
Na2  Na6 @  3.8 min 3.25 max 4  Na1 @  55 min  50 max  60
Na5  Na2 @  3.8 min 3.25 max 4  Na6 @  55 min  50 max  60  Na1 @  -180 min -190 max -170
Na3  Na5 @  3.8 min 3.25 max 4  Na2 @  55 min  50 max  60  Na6 @  -180 min -190 max -170
Na4  Na3 @  3.8 min 3.25 max 4  Na5 @  55 min  50 max  60  Na2 @  -180 min -190 max -170

C11  Na1 @ 0 min 2.6 max 2.9    Na6 @ 0 min 55 max 75      Na2 @ 0 min  105 max  125
O11  C11   1.265                Na1 @ 0 min 55 max 75      Na6 @ 0 min   10 max   50
C12  C11   1.550                O11   115.316              Na1 @ 0 min -220 max -140
O12  C11   1.265                C12   115.397              O11  -179.979
C13  C12   1.403                C11   120.820              O11    -0.064
C14  C13   1.398                C12   121.110              C11   179.988
C15  C14   1.400                C13   120.096              C12    -0.014
C16  C15   1.401                C14   119.356              C13     0.004
C17  C16   1.398                C15   120.127              C14    -0.015
H131 C13   1.092                C12   116.747              C11    -0.059
H141 C14   1.094                C13   120.178              C12  -179.961
H151 C15   1.093                C14   120.317              C13   179.938
H161 C16   1.094                C15   119.744              C14  -179.916
H171 C17   1.092                C16   122.070              C15  -179.997

C21  Na2 @ 0 min 2.6 max 2.9    Na4 @ 0 min 55 max 75      Na3 @ 0 min  105 max  125
O21  C21   1.265                Na2 @ 0 min 55 max 75      Na4 @ 0 min   10 max   50
C22  C21   1.550                O21   115.316              Na2 @ 0 min -220 max -140
O22  C21   1.265                C22   115.397              O21  -179.979
C23  C22   1.403                C21   120.820              O21    -0.064
C24  C23   1.398                C22   121.110              C21   179.988
C25  C24   1.400                C23   120.096              C22    -0.014
C26  C25   1.401                C24   119.356              C23     0.004
C27  C26   1.398                C25   120.127              C24    -0.015
H231 C23   1.092                C22   116.747              C21    -0.059
H241 C24   1.094                C23   120.178              C22  -179.961
H251 C25   1.093                C24   120.317              C23   179.938
H261 C26   1.094                C25   119.744              C24  -179.916
H271 C27   1.092                C26   122.070              C25  -179.997

C31  Na3 @ 0 min 2.6 max 2.9    Na5 @ 0 min 55 max 75      Na2 @ 0 min -125 max -105
O31  C31   1.265                Na3 @ 0 min 55 max 75      Na5 @ 0 min  135 max  150
C32  C31   1.550                O31   115.316              Na3 @ 0 min -220 max -140
O32  C31   1.265                C32   115.397              O31  -179.979
C33  C32   1.403                C31   120.820              O31    -0.064
C34  C33   1.398                C32   121.110              C31   179.988
C35  C34   1.400                C33   120.096              C32    -0.014
C36  C35   1.401                C34   119.356              C33     0.004
C37  C36   1.398                C35   120.127              C34    -0.015
H331 C33   1.092                C32   116.747              C31    -0.059
H341 C34   1.094                C33   120.178              C32  -179.961
H351 C35   1.093                C34   120.317              C33   179.938
H361 C36   1.094                C35   119.744              C34  -179.916
H371 C37   1.092                C36   122.070              C35  -179.997
```

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C41  Na4 @ 0 min 2.6 max 2.9    Na3 @ 0 min 55 max 75      Na5 @ 0 min -125 max -105
O41  C41   1.265               Na4 @ 0 min 55 max 75      Na3 @ 0 min  -40 max   -5
C42  C41   1.550                 O41   115.316             Na4 @ 0 min  140 max  220
O42  C41   1.265                 C42   115.397             O41  -179.979
C43  C42   1.403                 C41   120.820             O41    -0.064
C44  C43   1.398                 C42   121.110             C41   179.988
C45  C44   1.400                 C43   120.096             C42    -0.014
C46  C45   1.401                 C44   119.356             C43     0.004
C47  C46   1.398                 C45   120.127             C44    -0.015
H431 C43   1.092                 C42   116.747             C41    -0.059
H441 C44   1.094                 C43   120.178             C42  -179.961
H451 C45   1.093                 C44   120.317             C43   179.938
H461 C46   1.094                 C45   119.744             C44  -179.916
H471 C47   1.092                 C46   122.070             C45  -179.997

C51  Na5 @ 0 min 2.6 max 2.9    Na3 @ 0 min 55 max 75      Na4 @ 0 min  105 max  125
O51  C51   1.265               Na5 @ 0 min 55 max 75      Na3 @ 0 min   10 max   50
C52  C51   1.550                 O51   115.316             Na5 @ 0 min -220 max -140
O52  C51   1.265                 C52   115.397             O51  -179.979
C53  C52   1.403                 C51   120.820             O51    -0.064
C54  C53   1.398                 C52   121.110             C51   179.988
C55  C54   1.400                 C53   120.096             C52    -0.014
C56  C55   1.401                 C54   119.356             C53     0.004
C57  C56   1.398                 C55   120.127             C54    -0.015
H531 C53   1.092                 C52   116.747             C51    -0.059
H541 C54   1.094                 C53   120.178             C52  -179.961
H551 C55   1.093                 C54   120.317             C53   179.938
H561 C56   1.094                 C55   119.744             C54  -179.916
H571 C57   1.092                 C56   122.070             C55  -179.997

C61  Na6 @ 0 min 2.6 max 2.9    Na2 @ 0 min 55 max 75      Na3 @ 0 min  105 max  125
O61  C61   1.265               Na6 @ 0 min 55 max 75      Na2 @ 0 min   10 max   50
C62  C61   1.550                 O61   115.316             Na6 @ 0 min -220 max -140
O62  C61   1.265                 C62   115.397             O61  -179.979
C63  C62   1.403                 C61   120.820             O61    -0.064
C64  C63   1.398                 C62   121.110             C61   179.988
C65  C64   1.400                 C63   120.096             C62    -0.014
C66  C65   1.401                 C64   119.356             C63     0.004
C67  C66   1.398                 C65   120.127             C64    -0.015
H631 C63   1.092                 C62   116.747             C61    -0.059
H641 C64   1.094                 C63   120.178             C62  -179.961
H651 C65   1.093                 C64   120.317             C63   179.938
H661 C66   1.094                 C65   119.744             C64  -179.916
H671 C67   1.092                 C66   122.070             C65  -179.997
}

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