Electronic Supplementary Information

Non-zeolitic properties of the dipeptide _L-leucyl-_L-leucine as a result of the specific nanostructures formation

Marat A. Ziganshin,^{*,a} Aisylu S. Safiullina, ^a Sufia A. Ziganshina,^b Alexander V. Gerasimov, ^a Valery V. Gorbatchuk ^a

^a A.M. Butlerov Institute of Chemistry, Kazan Federal University, Kremlevskaya 18, Kazan, 420008 Russia, E-mail: Marat.Ziganshin@kpfu.ru ^b Kazan Zavoisky Physical-Technical Institute of the Kazan Scientific Center of the Russian Academy of Sciences, Sibirskii trakt 10/7, Kazan, 420029 Russia

- Experimental and calculated powder diffractograms;

- TG/DSC/MS data for the products of L-leucyl-L-leucine saturation with guest vapors;

- AFM images of the crystals obtained from a pyridine solution on the HOPG surface;

- SEM images of the initial film after saturation with vapor of dichloromethane and film obtained from a dichloromethane solution on the HOPG surface;

- Powder diffraction data.



Figure. **S1**. X-ray powder diffractograms for: (a) Leu-Leu•0.87H₂O clathrate calculated from single crystal X-ray data [Chem. Eur. J. 2001, V.7, P.5153], (b) initial powder of Leu-Leu used in present work.



Figure. **S2**.The data of TG/DSC/MS analysis for the sample of Leu-Leu heated up to 130°C and saturated with water vapor for 3 days at 298K. Heating rate is 10 K min⁻¹.



Figure. **S3**. The data of TG/DSC/MS analysis for the sample of Leu-Leu heated up to 180°C and stored at contact with water liquid water for 5 days at 298K. Heating rate is 10 K min⁻¹.



Figure. **S4**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of ethanol. Heating rate is 10 K min⁻¹.



Figure. **S5**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of *n*-propanol. Heating rate is 10 K min^{-1} .



Figure. **S6**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of isopropanol. Heating rate is 10 K min⁻¹.



Figure. **S7**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of *n*-buthanol. Heating rate is 10 K min^{-1} .



Figure. **S8**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of dichloromethane. Heating rate is 10 K min⁻¹.



Figure. **S9**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of tetrachloromethane. Heating rate is 10 K min⁻¹.



Figure. **S10**.The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of benzene. Heating rate is 10 K min⁻¹.



Figure. **S11**. The data of TG/DSC/MS analysis for the sample of Leu-Leu saturated with vapors of acetonitrile. Heating rate is 10 K min⁻¹.



Figure. **S12**. AFM image of the Leu-Leu film deposited on the HOPG from methanol solution after the saturation with ethanol vapors for 2 hour.



Figure. **S13**. 2D AFM images of the Leu-Leu crystals obtained from a pyridine solution on the HOPG surface, and cross-section by line.



Figure. S14. 3D AFM images of the Leu-Leu crystals obtained from a pyridine solution on the HOPG surface.



Figure. S15. AFM image of crystal which was formed on surface of Leu-Leu film after interaction with chloroform vapors.

Scanning electron microscopy

For scanning electron microscopy (SEM), films of dipeptide from methanol and dichloromethane solutions were prepared on the surfaces of HOPG as for AFM studies. The film from methanol solution was saturated with dichloromethane vapor for 200 min. SEM images were recorded using a scanning electron microscope Evo 50 (Carl Zeiss, Germany) at 20 kV.



Figure. S16. SEM image (20 kV) of Leu-Leu film deposited on HOPG from methanol solution and saturated with dichloromethane vapor for 200 min.



Figure. **S17**. SEM image (10 kV) of Leu-Leu film deposited on HOPG from dichloromethane solution.

1 $5.127(2)$ $17.221(8)$ 100 2 $5.741(3)$ $15.382(8)$ 61.3 3 $7.271(10)$ $12.148(17)$ 7.6 4 $9.296(8)$ $9.506(8)$ 5.8 5 $10.339(3)$ $8.549(2)$ 4.3 6 $11.569(7)$ $7.643(5)$ 85.7 7 $12.945(6)$ $6.833(3)$ 14.4 8 $13.945(5)$ $6.345(2)$ 3 9 $14.665(8)$ $6.035(3)$ 4.8 10 $15.52(3)$ $5.705(10)$ 2.3 11 $15.834(9)$ $5.592(3)$ 2.3 12 $16.437(4)$ $5.3886(13)$ 2.2 13 $17.405(10)$ $5.091(3)$ 5.9 14 $18.32(5)$ $4.840(12)$ 0.9 15 $18.7850(16)$ $4.7200(4)$ 47.5 16 $19.66(3)$ $4.511(6)$ 0.6 17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.30(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 20 $27.30(3)$ $3.264(3)$ 0.4 31 $27.30(3)$ $3.264(3)$ <t< th=""><th>№</th><th>2θ(deg)</th><th>d (Å)</th><th>Intensity</th></t<>	№	2θ (deg)	d (Å)	Intensity
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	5.127(2)	17.221(8)	100
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2	5.741(3)	15.382(8)	61.3
4 $9.296(8)$ $9.506(8)$ 5.8 5 $10.339(3)$ $8.549(2)$ 4.3 6 $11.569(7)$ $7.643(5)$ 85.7 7 $12.945(6)$ $6.833(3)$ 14.4 8 $13.945(5)$ $6.345(2)$ 3 9 $14.665(8)$ $6.035(3)$ 4.8 10 $15.52(3)$ $5.705(10)$ 2.3 11 $15.834(9)$ $5.592(3)$ 2.3 12 $16.437(4)$ $5.3886(13)$ 2.2 13 $17.405(10)$ $5.091(3)$ 5.9 14 $18.32(5)$ $4.840(12)$ 0.9 15 $18.7850(16)$ $4.7200(4)$ 47.5 16 $19.66(3)$ $4.511(6)$ 0.6 17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ <td>3</td> <td>7.271(10)</td> <td>12.148(17)</td> <td>7.6</td>	3	7.271(10)	12.148(17)	7.6
5 $10.339(3)$ $8.549(2)$ 4.3 6 $11.569(7)$ $7.643(5)$ 85.7 7 $12.945(6)$ $6.833(3)$ 14.4 8 $13.945(5)$ $6.345(2)$ 3 9 $14.665(8)$ $6.035(3)$ 4.8 10 $15.52(3)$ $5.705(10)$ 2.3 11 $15.834(9)$ $5.592(3)$ 2.3 12 $16.437(4)$ $5.3886(13)$ 2.2 13 $17.405(10)$ $5.091(3)$ 5.9 14 $18.32(5)$ $4.840(12)$ 0.9 15 $18.7850(16)$ $4.7200(4)$ 47.5 16 $19.66(3)$ $4.511(6)$ 0.6 17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$	4	9.296(8)	9.506(8)	5.8
611.569(7)7.643(5)85.7712.945(6) $6.833(3)$ 14.4813.945(5) $6.345(2)$ 3914.665(8) $6.035(3)$ 4.81015.52(3) $5.705(10)$ 2.31115.834(9) $5.592(3)$ 2.31216.437(4) $5.3886(13)$ 2.21317.405(10) $5.091(3)$ 5.9 1418.32(5) $4.840(12)$ 0.9 1518.7850(16) $4.7200(4)$ 47.5 1619.66(3) $4.511(6)$ 0.6 1720.376(6) $4.3548(12)$ 6.6 1821.077(3) $4.2117(6)$ 211921.543(6) $4.1215(11)$ 7.3 2022.330(7) $3.9781(13)$ 7.2 2123.419(11) $3.7956(17)$ 1.9 2224.101(4) $3.6897(5)$ 9.1 2324.640(15) $3.610(2)$ 0.5 2424.780(14) $3.5901(19)$ 1.7 2525.12(2) $3.542(3)$ 0.9 2625.802(15) $3.450(2)$ 0.5 2726.298(14) $3.3861(18)$ 4.5 2826.44(2) $3.368(3)$ 5.2 2926.744(7) $3.3307(9)$ 3.2 3027.30(3) $3.264(3)$ 0.4 3127.88(4) $3.197(4)$ 0.2 3228.380(7) $3.1423(8)$ 1.8 3329.36(2) $2.589(18)$ 1.3 3731.638(16) $2.8258(14)$	5	10.339(3)	8.549(2)	4.3
7 $12.945(6)$ $6.833(3)$ 14.4 8 $13.945(5)$ $6.345(2)$ 3 9 $14.665(8)$ $6.035(3)$ 4.8 10 $15.52(3)$ $5.705(10)$ 2.3 11 $15.834(9)$ $5.592(3)$ 2.3 12 $16.437(4)$ $5.3886(13)$ 2.2 13 $17.405(10)$ $5.091(3)$ 5.9 14 $18.32(5)$ $4.840(12)$ 0.9 15 $18.7850(16)$ $4.7200(4)$ 47.5 16 $19.66(3)$ $4.511(6)$ 0.6 17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(1$	6	11.569(7)	7.643(5)	85.7
8 $13.945(5)$ $6.345(2)$ 3 9 $14.665(8)$ $6.035(3)$ 4.8 10 $15.52(3)$ $5.705(10)$ 2.3 11 $15.834(9)$ $5.592(3)$ 2.3 12 $16.437(4)$ $5.3886(13)$ 2.2 13 $17.405(10)$ $5.091(3)$ 5.9 14 $18.32(5)$ $4.840(12)$ 0.9 15 $18.7850(16)$ $4.7200(4)$ 47.5 16 $19.66(3)$ $4.511(6)$ 0.6 17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ 2.8589	7	12.945(6)	6.833(3)	14.4
9 $14.665(8)$ $6.035(3)$ 4.8 10 $15.52(3)$ $5.705(10)$ 2.3 11 $15.834(9)$ $5.592(3)$ 2.3 12 $16.437(4)$ $5.3886(13)$ 2.2 13 $17.405(10)$ $5.091(3)$ 5.9 14 $18.32(5)$ $4.840(12)$ 0.9 15 $18.7850(16)$ $4.7200(4)$ 47.5 16 $19.66(3)$ $4.511(6)$ 0.6 17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9858(14)$ 2.8 38 $32.086(7)$ 2	8	13.945(5)	6.345(2)	3
1015.52(3)5.705(10)2.31115.834(9)5.592(3)2.31216.437(4)5.3886(13)2.21317.405(10)5.091(3)5.91418.32(5)4.840(12)0.91518.7850(16)4.7200(4)47.51619.66(3)4.511(6)0.61720.376(6)4.3548(12)6.61821.077(3)4.2117(6)211921.543(6)4.1215(11)7.32022.330(7)3.9781(13)7.22123.419(11)3.7956(17)1.92224.101(4)3.6897(5)9.12324.640(15)3.610(2)0.52424.780(14)3.5901(19)1.72525.12(2)3.542(3)0.92625.802(15)3.450(2)0.52726.298(14)3.3861(18)4.52826.44(2)3.368(3)5.22926.744(7)3.3307(9)3.23027.30(3)3.264(3)0.43127.88(4)3.197(4)0.23228.380(7)3.1423(8)1.83329.36(2)3.040(2)0.93429.742(16)3.0015(16)1.53530.782(12)2.9024(11)1.93631.26(2)2.8589(18)1.33731.638(16)2.8258(14)2.83832.086(7)2.7873(6)5.33932.636(9)2.711(4)0.3	9	14.665(8)	6.035(3)	4.8
11 $15.834(9)$ $5.592(3)$ 2.3 12 $16.437(4)$ $5.3886(13)$ 2.2 13 $17.405(10)$ $5.091(3)$ 5.9 14 $18.32(5)$ $4.840(12)$ 0.9 15 $18.7850(16)$ $4.7200(4)$ 47.5 16 $19.66(3)$ $4.511(6)$ 0.6 17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 20 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$	10	15.52(3)	5.705(10)	2.3
12 $16.437(4)$ $5.3886(13)$ 2.2 13 $17.405(10)$ $5.091(3)$ 5.9 14 $18.32(5)$ $4.840(12)$ 0.9 15 $18.7850(16)$ $4.7200(4)$ 47.5 16 $19.66(3)$ $4.511(6)$ 0.6 17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ <td>11</td> <td>15.834(9)</td> <td>5.592(3)</td> <td>2.3</td>	11	15.834(9)	5.592(3)	2.3
13 $17.405(10)$ $5.091(3)$ 5.9 14 $18.32(5)$ $4.840(12)$ 0.9 15 $18.7850(16)$ $4.7200(4)$ 47.5 16 $19.66(3)$ $4.511(6)$ 0.6 17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.7111(4)$ 0.3 41 $33.396(12)$	12	16.437(4)	5.3886(13)	2.2
14 $18.32(5)$ $4.840(12)$ 0.9 15 $18.7850(16)$ $4.7200(4)$ 47.5 16 $19.66(3)$ $4.511(6)$ 0.6 17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ <t< td=""><td>13</td><td>17.405(10)</td><td>5.091(3)</td><td>5.9</td></t<>	13	17.405(10)	5.091(3)	5.9
15 $18.7850(16)$ $4.7200(4)$ 47.5 16 $19.66(3)$ $4.511(6)$ 0.6 17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6580(19)$ 0.7 45 $35.08(2)$	14	18.32(5)	4.840(12)	0.9
16 $19.66(3)$ $4.511(6)$ 0.6 17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ $3.$	15	18.7850(16)	4.7200(4)	47.5
17 $20.376(6)$ $4.3548(12)$ 6.6 18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ <td< td=""><td>16</td><td>19.66(3)</td><td>4.511(6)</td><td>0.6</td></td<>	16	19.66(3)	4.511(6)	0.6
18 $21.077(3)$ $4.2117(6)$ 21 19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.63809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$	17	20.376(6)	4.3548(12)	6.6
19 $21.543(6)$ $4.1215(11)$ 7.3 20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.66068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4709(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 49 $36.79(2)$ <td>18</td> <td>21.077(3)</td> <td>4.2117(6)</td> <td>21</td>	18	21.077(3)	4.2117(6)	21
20 $22.330(7)$ $3.9781(13)$ 7.2 21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.44709(13)$ <	19	21.543(6)	4.1215(11)	7.3
21 $23.419(11)$ $3.7956(17)$ 1.9 22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4408(13)$ 0.7 48 $36.33(2)$	20	22.330(7)	3.9781(13)	7.2
22 $24.101(4)$ $3.6897(5)$ 9.1 23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4408(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$	21	23.419(11)	3.7956(17)	1.9
23 $24.640(15)$ $3.610(2)$ 0.5 24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4970(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$ 3.8 51 $37.909(14)$	22	24.101(4)	3.6897(5)	9.1
24 $24.780(14)$ $3.5901(19)$ 1.7 25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4970(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$ 3.8 51 $37.909(14)$ $2.3715(9)$	23	24.640(15)	3.610(2)	0.5
25 $25.12(2)$ $3.542(3)$ 0.9 26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4970(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$ 3.8 51 $37.909(14)$ $2.3715(9)$ 1.9 52 $38.31(3)$ $2.3476(17)$ 0	24	24.780(14)	3.5901(19)	1.7
26 $25.802(15)$ $3.450(2)$ 0.5 27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4970(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$ 3.8 51 $37.909(14)$ $2.3715(9)$ 1.9 52 $38.31(3)$ $2.3476(17)$ 0.4	25	25.12(2)	3.542(3)	0.9
27 $26.298(14)$ $3.3861(18)$ 4.5 28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4970(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$ 3.8 51 $37.909(14)$ $2.3715(9)$ 1.9 52 $38.31(3)$ $2.3476(17)$ 0.4	26	25.802(15)	3.450(2)	0.5
28 $26.44(2)$ $3.368(3)$ 5.2 29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4970(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$ 3.8 51 $37.909(14)$ $2.3715(9)$ 1.9 52 $38.31(3)$ $2.3476(17)$ 0.4	27	26.298(14)	3.3861(18)	4.5
29 $26.744(7)$ $3.3307(9)$ 3.2 30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4970(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$ 3.8 51 $37.909(14)$ $2.3715(9)$ 1.9 52 $38.31(3)$ $2.3476(17)$ 0.4	28	26.44(2)	3.368(3)	5.2
30 $27.30(3)$ $3.264(3)$ 0.4 31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4970(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$ 3.8 51 $37.909(14)$ $2.3715(9)$ 1.9 52 $38.31(3)$ $2.3476(17)$ 0.4	29	26.744(7)	3.3307(9)	3.2
31 $27.88(4)$ $3.197(4)$ 0.2 32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4970(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$ 3.8 51 $37.909(14)$ $2.3715(9)$ 1.9 52 $38.31(3)$ $2.3476(17)$ 0.4	30	27.30(3)	3.264(3)	0.4
32 $28.380(7)$ $3.1423(8)$ 1.8 33 $29.36(2)$ $3.040(2)$ 0.9 34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4970(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$ 3.8 51 $37.909(14)$ $2.3715(9)$ 1.9 52 $38.31(3)$ $2.3476(17)$ 0.4	31	27.88(4)	3.197(4)	0.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32	28.380(7)	3.1423(8)	1.8
34 $29.742(16)$ $3.0015(16)$ 1.5 35 $30.782(12)$ $2.9024(11)$ 1.9 36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4970(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$ 3.8 51 $37.909(14)$ $2.3715(9)$ 1.9 52 $38.31(3)$ $2.3476(17)$ 0.4	33	29.36(2)	3.040(2)	0.9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	34	29.742(16)	3.0015(16)	1.5
36 $31.26(2)$ $2.8589(18)$ 1.3 37 $31.638(16)$ $2.8258(14)$ 2.8 38 $32.086(7)$ $2.7873(6)$ 5.3 39 $32.636(9)$ $2.7415(7)$ 3.1 40 $33.02(5)$ $2.711(4)$ 0.3 41 $33.396(12)$ $2.6809(9)$ 3 42 $33.76(4)$ $2.653(3)$ 3.3 43 $33.882(13)$ $2.6435(10)$ 2.8 44 $34.37(3)$ $2.6068(19)$ 0.7 45 $35.08(2)$ $2.5556(15)$ 0.4 46 $35.52(2)$ $2.5253(15)$ 0.9 47 $35.937(19)$ $2.4970(13)$ 1.7 48 $36.33(2)$ $2.4709(13)$ 0.7 50 $37.507(9)$ $2.3960(5)$ 3.8 51 $37.909(14)$ $2.3715(9)$ 1.9 52 $38.31(3)$ $2.3476(17)$ 0.4	35	30.782(12)	2.9024(11)	1.9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	36	31.26(2)	2.8589(18)	1.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	37	31.638(16)	2.8258(14)	2.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	38	32.086(7)	2.7873(6)	5.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	39	32.636(9)	2.7415(7)	3.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	40	33.02(5)	2.711(4)	0.3
$\begin{array}{cccccccc} 42 & 33.76(4) & 2.653(3) & 3.3 \\ 43 & 33.882(13) & 2.6435(10) & 2.8 \\ 44 & 34.37(3) & 2.6068(19) & 0.7 \\ 45 & 35.08(2) & 2.5556(15) & 0.4 \\ 46 & 35.52(2) & 2.5253(15) & 0.9 \\ 47 & 35.937(19) & 2.4970(13) & 1.7 \\ 48 & 36.33(2) & 2.4709(13) & 0.9 \\ 49 & 36.79(2) & 2.4408(13) & 0.7 \\ 50 & 37.507(9) & 2.3960(5) & 3.8 \\ 51 & 37.909(14) & 2.3715(9) & 1.9 \\ 52 & 38.31(3) & 2.3476(17) & 0.4 \\ \end{array}$	41	33.396(12)	2.6809(9)	3
4333.882(13)2.6435(10)2.84434.37(3)2.6068(19)0.74535.08(2)2.5556(15)0.44635.52(2)2.5253(15)0.94735.937(19)2.4970(13)1.74836.33(2)2.4709(13)0.94936.79(2)2.4408(13)0.75037.507(9)2.3960(5)3.85137.909(14)2.3715(9)1.95238.31(3)2.3476(17)0.4	42	33.76(4)	2.653(3)	3.3
4434.37(3)2.6068(19)0.74535.08(2)2.5556(15)0.44635.52(2)2.5253(15)0.94735.937(19)2.4970(13)1.74836.33(2)2.4709(13)0.94936.79(2)2.4408(13)0.75037.507(9)2.3960(5)3.85137.909(14)2.3715(9)1.95238.31(3)2.3476(17)0.4	43	33.882(13)	2.6435(10)	2.8
4535.08(2)2.5556(15)0.44635.52(2)2.5253(15)0.94735.937(19)2.4970(13)1.74836.33(2)2.4709(13)0.94936.79(2)2.4408(13)0.75037.507(9)2.3960(5)3.85137.909(14)2.3715(9)1.95238.31(3)2.3476(17)0.4	44	34.37(3)	2.6068(19)	0.7
4635.52(2)2.5253(15)0.94735.937(19)2.4970(13)1.74836.33(2)2.4709(13)0.94936.79(2)2.4408(13)0.75037.507(9)2.3960(5)3.85137.909(14)2.3715(9)1.95238.31(3)2.3476(17)0.4	45	35.08(2)	2.5556(15)	0.4
4735.937(19)2.4970(13)1.74836.33(2)2.4709(13)0.94936.79(2)2.4408(13)0.75037.507(9)2.3960(5)3.85137.909(14)2.3715(9)1.95238.31(3)2.3476(17)0.4	46	35.52(2)	2.5253(15)	0.9
4836.33(2)2.4709(13)0.94936.79(2)2.4408(13)0.75037.507(9)2.3960(5)3.85137.909(14)2.3715(9)1.95238.31(3)2.3476(17)0.4	47	35.937(19)	2.4970(13)	1.7
4936.79(2)2.4408(13)0.75037.507(9)2.3960(5)3.85137.909(14)2.3715(9)1.95238.31(3)2.3476(17)0.4	48	36.33(2)	2.4709(13)	0.9
5037.507(9)2.3960(5)3.85137.909(14)2.3715(9)1.95238.31(3)2.3476(17)0.4	49	36.79(2)	2.4408(13)	0.7
5137.909(14)2.3715(9)1.95238.31(3)2.3476(17)0.4	50	37.507(9)	2.3960(5)	3.8
52 38.31(3) 2.3476(17) 0.4	51	37.909(14)	2.3715(9)	1.9
	52	38.31(3)	2.3476(17)	0.4

 Table. S1. Powder diffraction data of Leu-Leu initial powder.

53	38.690(13)	2.3254(8)	1.7
54	39.459(14)	2.2818(8)	1.4
55	39.88(3)	2.2589(17)	0.2

Table. S2. Powder diffraction data of Leu-Leu sample after heating up to 130°C.

N⁰	2θ (deg)	d (Å)	Intensity
1	6.852(6)	12.889(12)	100
2	6.9(6)	12.8(10)	7.4
3	7.115(6)	12.414(10)	35.5
4	7.785(6)	11.348(9)	53.9
5	13.524(16)	6.542(8)	6
6	14.03(2)	6.308(10)	2.3
7	17.319(10)	5.116(3)	8.5
8	18.61(3)	4.765(7)	4.7
9	20.51(2)	4.327(5)	4
10	24.20(4)	3.675(6)	1.9
11	32.78(19)	2.730(15)	0.6

Table. S3. Powder diffraction data of Leu-Leu sample after heating up to 130°C and saturated with vapors of water for 3 days at rt.

N₂	2θ (deg)	<i>d</i> (A)	Intensity
1	4.183(9)	21.11(5)	3
2	5.0274(11)	17.563(4)	100
3	5.6476(19)	15.636(5)	51.5
4	7.180(6)	12.302(10)	8.5
5	8.492(10)	10.404(12)	1.6
6	9.221(4)	9.583(4)	4.4
7	10.2632(10)	8.6121(9)	58.5
8	11.4956(17)	7.6915(12)	11.8
9	12.885(3)	6.8651(13)	1.7
10	13.8916(14)	6.3698(6)	3.4
11	14.614(4)	6.0565(15)	1.5
12	15.491(6)	5.715(2)	1.4
13	15.753(5)	5.6209(16)	1.1
14	16.378(3)	5.4079(10)	4
15	17.258(18)	5.134(5)	1.4
16	18.16(4)	4.880(10)	1.9
17	18.730(3)	4.7338(7)	31.8
18	19.59(3)	4.527(7)	1.3
19	20.338(11)	4.363(2)	4.8
20	21.005(8)	4.2259(15)	13.4
21	21.470(12)	4.135(2)	4.6
22	22.288(15)	3.986(3)	3.5
23	23.362(8)	3.8046(13)	1.5
24	24.053(2)	3.6969(3)	7.2
25	24.660(5)	3.6072(8)	1.1
26	25.060(7)	3.5506(10)	0.9
27	25.728(13)	3.4598(17)	0.6
28	26.144(4)	3.4057(6)	1.1
29	26.299(4)	3.3860(5)	5.6

30	26.684(4)	3.3381(5)	2.3
31	27.228(17)	3.273(2)	0.5
32	27.85(2)	3.201(3)	0.3
33	28.345(6)	3.1461(6)	1.2
34	29.339(17)	3.0417(18)	0.6
35	29.720(13)	3.0036(13)	1
36	30.746(9)	2.9057(8)	1.5
37	31.224(15)	2.8623(13)	1
38	31.589(10)	2.8300(9)	1.8
39	32.042(5)	2.7911(4)	3.3
40	32.592(7)	2.7452(6)	2
41	32.92(4)	2.718(3)	0.4
42	33.336(8)	2.6856(6)	1.9
43	33.762(4)	2.6527(3)	4.3
44	34.327(19)	2.6103(14)	0.4
45	35.04(3)	2.559(2)	0.3
46	35.503(18)	2.5264(13)	0.5
47	35.902(15)	2.4993(10)	1
48	36.286(16)	2.4737(10)	0.6
49	36.784(17)	2.4414(11)	0.2
50	37.465(4)	2.3986(3)	2
51	37.904(8)	2.3718(5)	1.3
52	38.29(2)	2.3489(14)	0.4
53	38.614(8)	2.3298(5)	1
54	39.423(13)	2.2838(7)	1
55	39.82(3)	2.2620(15)	0.2

Table. S4. Powder diffraction data of Leu-Leu sample after heating up to 180°.

N⁰	2θ (deg)	d (Å)	Intensity
1	6.989(6)	12.638(10)	100
2	14.00(3)	6.323(16)	1.5
3	16.58(5)	5.344(16)	1.5
4	18.00(13)	4.93(4)	3.3
5	18.87(11)	4.70(3)	2.9
6	20.71(6)	4.285(13)	2.6
7	27.5(2)	3.24(3)	0.5
8	31.5(3)	2.84(3)	1.1

Table. S5. Powder diffraction data of Leu-Leu sample after heating up to 180° and saturated with liquid water for 5 days at rt.

N⁰	2θ (deg)	d (Å)	Intensity
1	7.037(6)	12.552(10)	100
2	12.39(3)	7.137(15)	1.9
3	14.03(4)	6.308(18)	3.4
4	16.62(3)	5.331(10)	3.7
5	17.9(2)	4.95(6)	2.6
6	18.83(7)	4.709(17)	13.8
7	20.69(7)	4.290(14)	6.8
8	23.6(2)	3.77(4)	1.9
9	31.82(15)	2.810(13)	1.8