Electronic Supplementary Information

For

Identification of incommensurability in L-Leucine ; are lattice instabilities can be considered as general phenomena in hydrophobic amino acids?

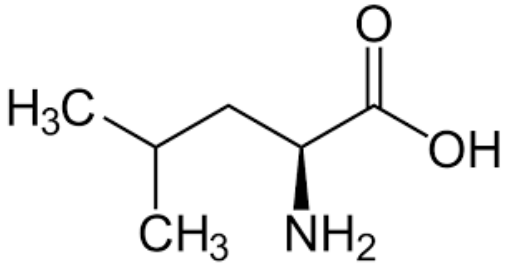
Yannick Guinet, Laurent Paccou, Florence Danède, Patrick Derollez and Alain Hédoux*

Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France

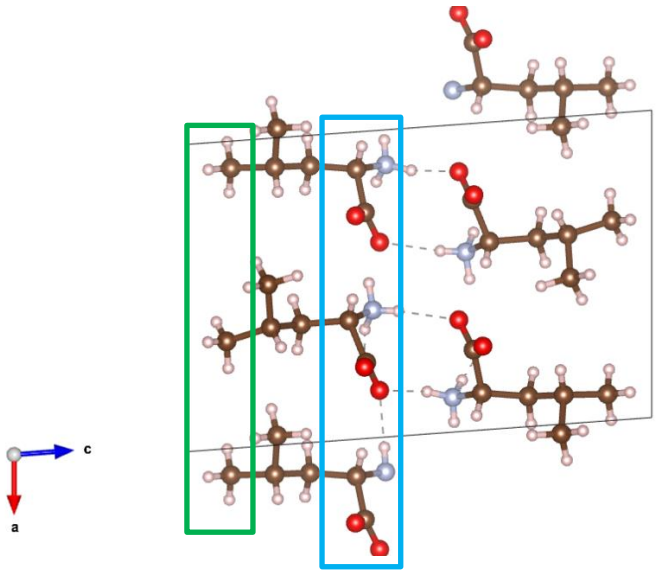
*corresponding author : alain.hedoux@univ-lille.fr

- Figure S1: Structural descriptions of L-leucine and L-norleucine
- Figure S2: Description of the fitting procedure of the low-frequency Raman
- Figure S3: Description of the fitting procedure of the high-frequency Raman spectrum (C – H stretching mode region)
- Figure S4: Description of the refinements of the X-Ray powder diffraction patterns at 293 K and 373 K.
- Table S1: Results of the refinements of the X-Ray powder diffraction data

L-Leucine

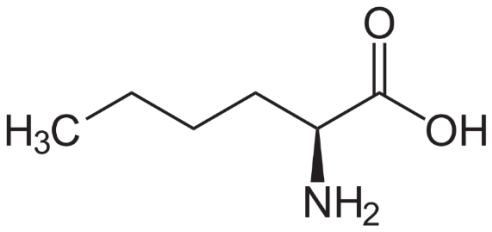


a) Chemical structure

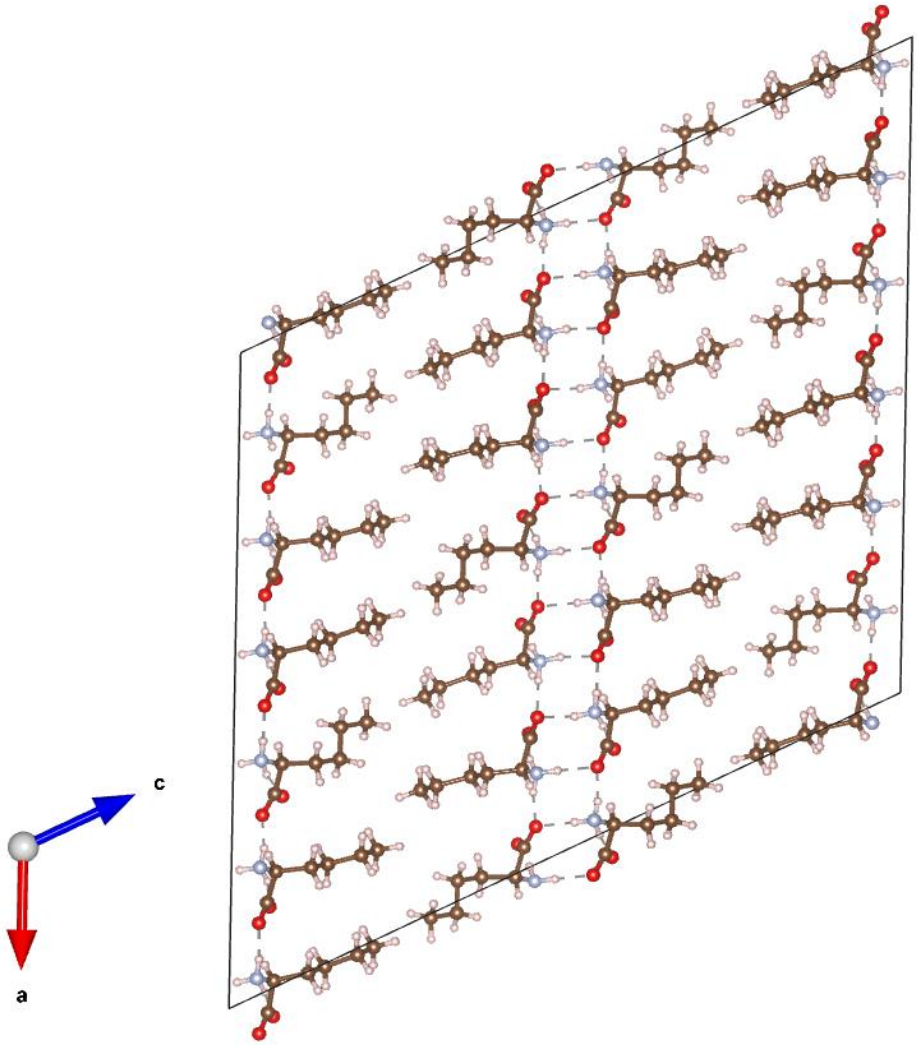


b) Unit cell of L-Leucine at 120 K from data of C. Görbitz and B. Dalhus obtained. Dashed lines indicate H-bonds (*Acta Cryst* **1996,** *C52*, 1754-1756).The green frame localizes the hydrophobic layer and the blue localizes the hydrophilic layer

L-Norleucine



c) Chemical structure



d) Unit cell of L-Norleucine at 210 K from data of C. Görbitz et al., IUCrj (2016), 3, 341-353.

Figure S1: conformational and Crystallographic structure of L-leucine and L-Norleucine

Low-frequency Raman spectroscopy

The low-frequency Raman intensity $I_{Raman}(\omega, T)$ was transformed into reduced intensity $I_r(\omega)$ for correcting the spectrum distortion from temperature fluctuation according to:

$$I_r(\omega) = \frac{I_{Raman}(\omega, T)}{[n(\omega, T) + 1]\omega}$$

where $n(\omega, T)$ is the Bose-Einstein factor.

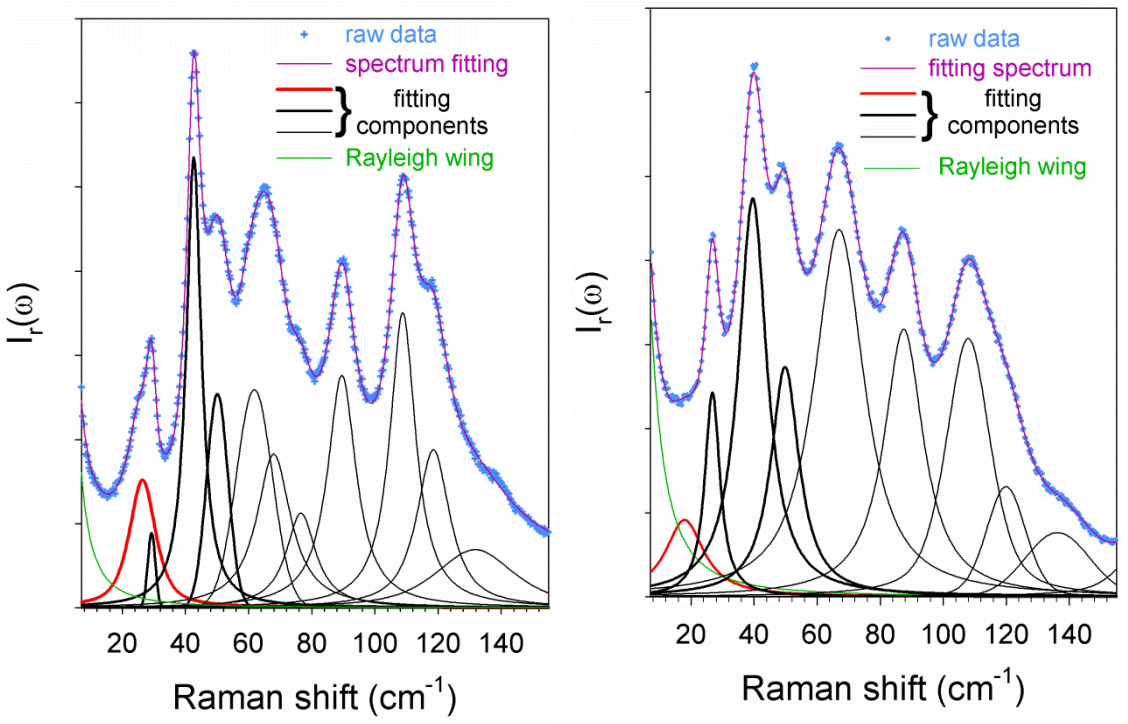


Figure S2: fitting procedure of the low-frequency Raman spectrum collected at T= 220 K (left) and 320 K (right). The green component represents the Rayleigh wing which appears broadened at 320 K. The frequency temperature dependence of the four bands in thick line are presented in the manuscript, including the band plotted in red corresponding to the soft mode. The components are mixed Gaussian-Lorentzian functions except the Rayleigh wing usually fitted by a Lorentzian shape fixed at ω= 0.

Analysis of the high-frequency spectrum, mainly composed of C – H stretching bands in the 2800 – 3050 spectral range.

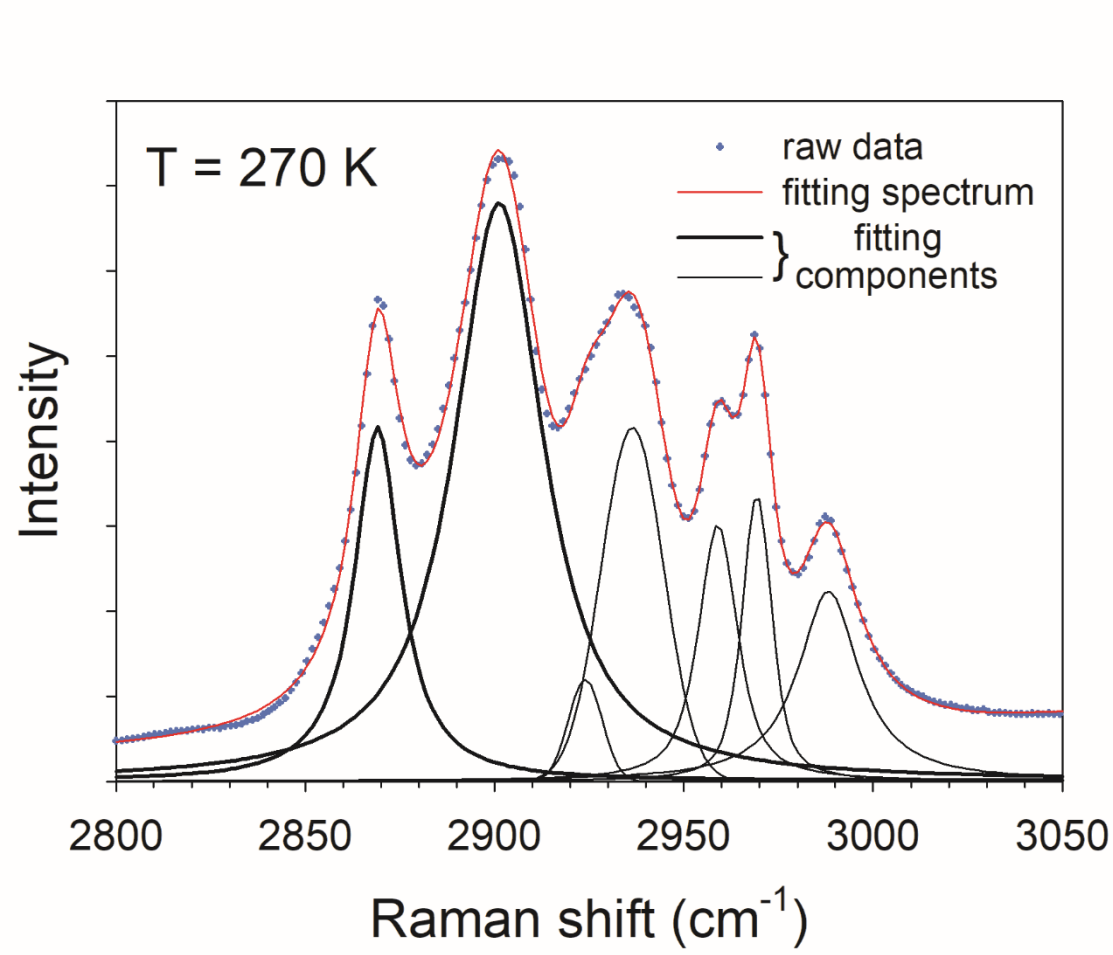


Figure S3: Fitting procedure of the C – H stretching spectrum at 270 K. The frequency temperature dependence of the two bands plotted in thick line are presented in the manuscript. The components are mixed Gaussian-Lorentzian functions.

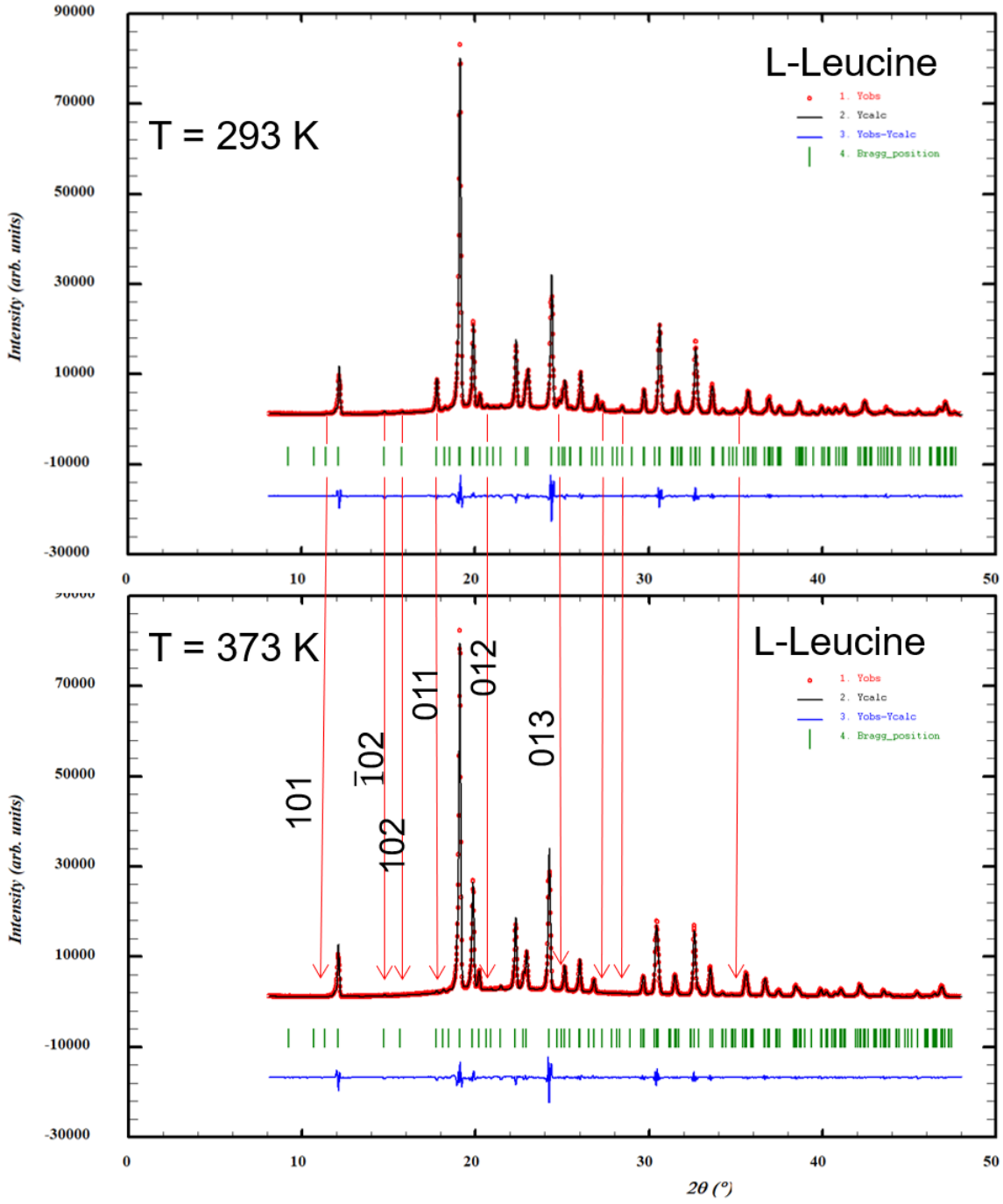


Figure S4: Results of Le Bail refinements at 293 K and 373 K. Arrows show weakly intense X-ray reflections detected at room temperature and vanishing at 373 K. They are indexed (as Bragg peaks) with the cell parameters reported in Table 1 in Supporting Information.

Crystalographic data for L-Leucine obtained after Le Bail refinement	T = 293 K	T = 373 K
Crystal data		
Chemical formula	$C_6H_{13}NO_2$	$C_6H_{13}NO_2$
M	131.17	131.17
Crystal system, space group	Monoclinic, $P2_1$	Monoclinic, $P2_1$
a, b, c (Å)	9.59361(37), 5.30459(35), 14.61713(54),	9.62060(41), 5.31610(32), 14.70357(54)
α, β, Y (°)	90, 93,9744(33), 90	90, 93.6569(32), 90
V ($Å^3$)	742.05	750.67
Z	2	2
Radiation type	X-Rays, λ_1=1.54056 Å	X-Rays, λ_1=1.54056 Å
Specimen shape, size (mm)	Cylinder, 0.7	Cylinder, 0.7
2θ (°)	3 – 60	3 – 60
Data collection		
Diffractometer	X'Pert Panalytical	X'Pert Panalytical
Specimen mounting	0.7 mm diameter Lindemann capillary	0.7 mm diameter Lindemann capillary
Data collection mode	transmission	transmission
Scan method	linear detector	linear detector
Step size (° 2θ)	0.0167	0.0167
Refinement		
R factors not corrected for backgroiund	R_p=0.0481, R_{wp}=0.0695, R_{exp}=0.0188	R_p=0.0449, R_{wp}=0.0650, R_{exp}=0.0188
No of profile data step	3410	3410
No of contributing reflections	144	144
No of fitted parameters	23	23

Table S1: Results of XRPD pattern refinements with Le Bail method in the Fullprof program.