Supplementary information

Studies on the internal medium-range ordering and high pressure dynamics in modified ibuprofens

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XRD data

The diffraction pattern of crystalline ibuprofen at 293 K from 1 to 22° scattering angles 2Θ was refined using Le Bail's method[1] in the FULLPROF program.[2] The Pseudo-Voigt function was used to fit the Bragg peaks. Instrumental resolution parameters U, V, W were determined for Si NIST 640e standard. The background was fitted with the polynomial function of the 3rd degree. The other refined parameters were as follows: scale factor, lattice parameters a, b, c, zero shift, peak asymmetry parameter, temperature factors B, and broadening line parameters X, Y. At the end of the refinement with P 21/c space group the conventional reliability factors were as follows: R_p = 7.89%, R_{wp} = 9.95%, R_{exp} = 28.85%, χ^2 = 12.1%; the values of the lattice parameters were: a = 14.5779(9), b = 7.8676(0), c = 10.6836(3) Å, volume

V = 1209.09 (5) Å^3, density d = 1.113 g/cm^3. The Rietveld fit to the diffraction pattern is shown in Fig. S1.

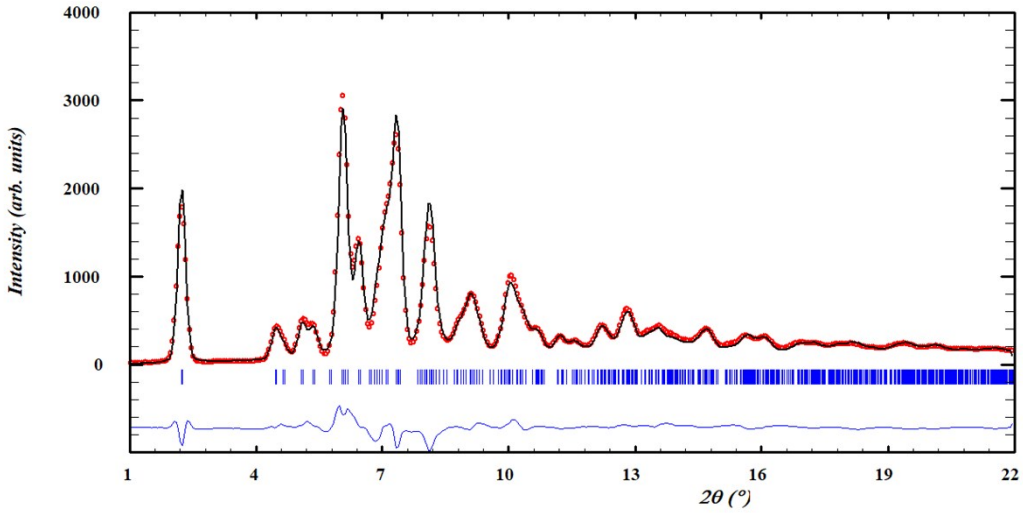
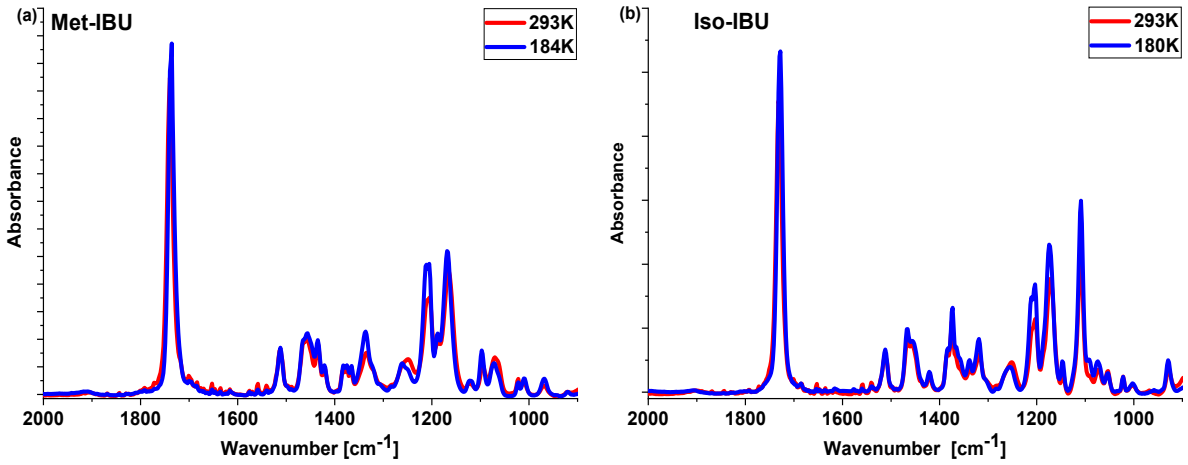


Fig. S1. The Rietveld refinement of the crystalline ibuprofen phase at 293 K. The observed intensities are indicated by red dots, the fit is a black line, and the difference function is a blue line. The vertical bars correspond to the positions of the Bragg peaks.

FTIR data



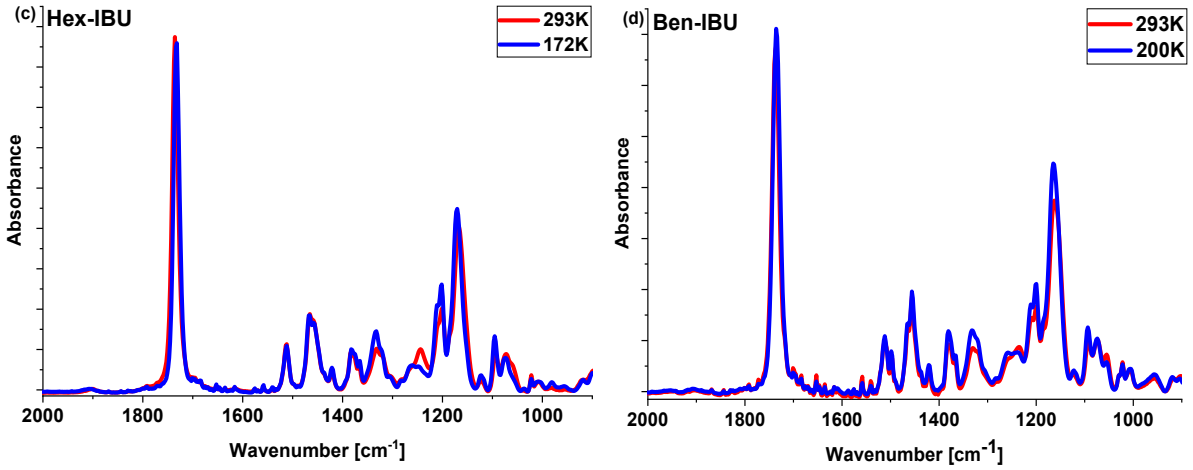


Fig. S2. Infrared spectra of investigated esters measured at T=293 K and the glass transition temperature of each sample in the 2000-900 cm^{-1} frequency range.

BDS data

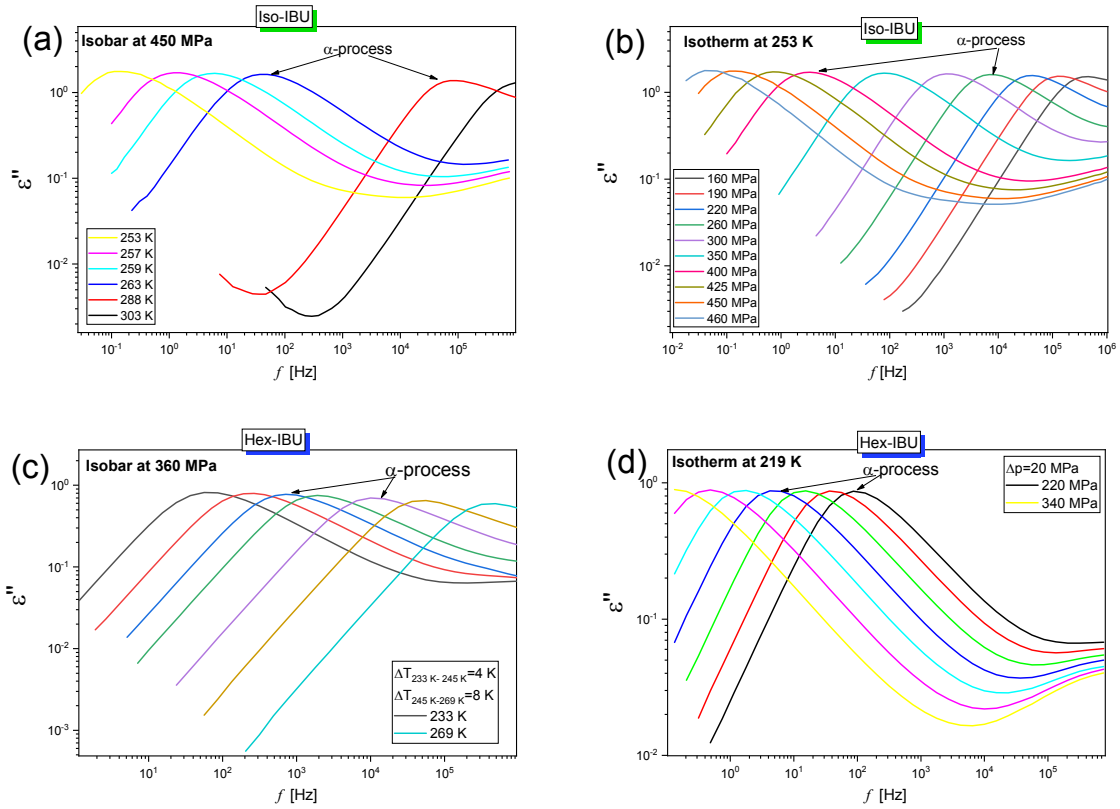


Fig. S3. Representative dielectric loss spectra measured for Iso-IBU (a,b) and Hex-IBU (c,d) at indicated thermodynamic conditions.

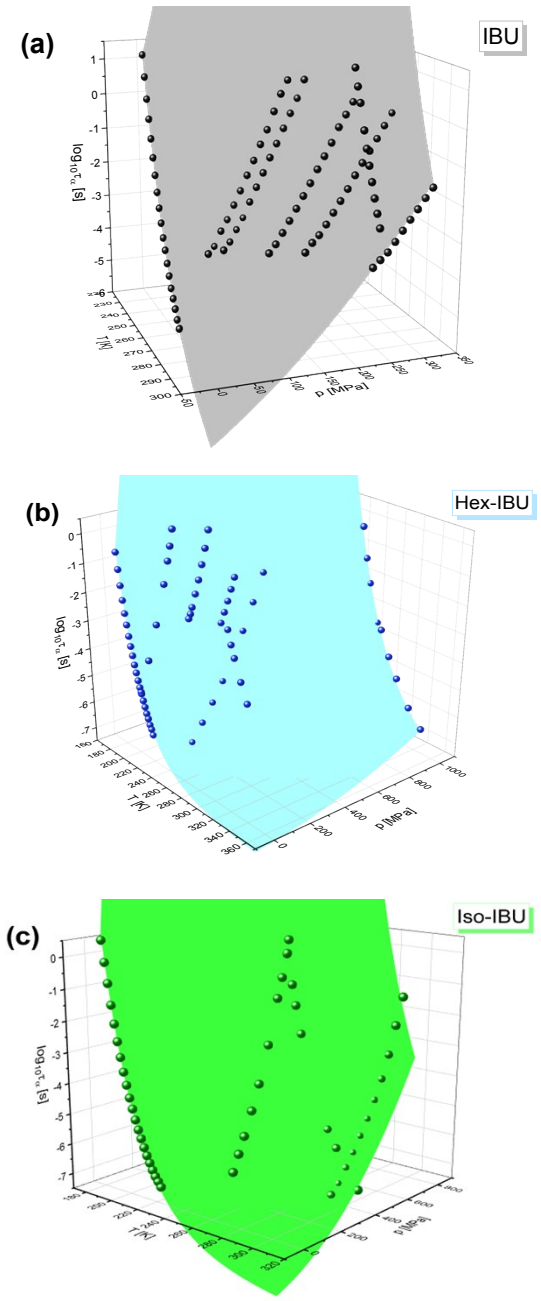


Fig. S4. α-relaxation times of IBU (a), Hex-IBU (b), and Iso-IBU (c) plotted versus temperature (T) and pressure (p). Grey, blue, and green areas represent surface fits to Avramov equation (Eq. 2). Data for native IBU were taken from Ref. [3].

References

1 A. Le Bail, H. Duroy, J. L. Fourquet, *Mater. Res. Bull.,* 1988, **23**, 447–452.
2 J. Rodriguez-Carvajal, FULLPROF, Version 1.9c. LLB, CEA/Saclay, France, 2001.
3 K. Adrjanowicz, Z. Wojnarowska, M. Paluch, J. Pionteck, *J. Phys. Chem. B,* 2011, **115**, 4559–4567.