Synergetic effect of temperature and pressure on energetic and structural characteristics of {ZIF-8 + water} molecular spring

Ya. Grosu ^{a,b,c}, G. Renaudin ^{a,b}, V. Eroshenko ^c, J.-M. Nedelec ^{a,b}, J.-P.E. Grolier ^{a,b}

^{*a*} Clermont University ENSCCF, Institute of Chemistry of Clermont-Ferrand, BP 10448, 63000 Clermont-Ferrand, France.

^b CNRS, UMR 6296, ICCF, 24 av. des Landais, 63171 Aubière, France.

^{*c*} Laboratory of Thermomolecular Energetics, National Technical University of Ukraine "Kyiv Polytechnic Institute", Prospect Peremogy 37, 03056 Kyiv, Ukraine.

Corresponding Author: eroshenko@kpi.ua

Supplementary information

Scheme 1S. The calorimeter setup.



Т,К	275	300	310	320	330	340	350	360
W_{int} [J g ⁻¹]	8.8	9.6	9.8	9.9	9.9	9.9	9.8	9.5
W_{ext} [J g ⁻¹]	5.7	7.0	7.5	7.9	8.2	8.4	8.4	8.3
Q_{int} [J g ⁻¹]		4.4	7.4	9.4	14.4	13	26.3	
Q_{ext} [J g ⁻¹]			5.4	6.3	12.7	12.9	25.7	
P _{int} [MPa]	23.0	24.6	25.3	25.8	26.0	25.9	25.5	24.9
$P_{ext}(1^{st} \text{ peak})[\text{MPa}]$	18.8	21.8	22.5	23.0	22.9	22.2	22.3	21.9
P_{ext2} (2 nd peak) [MPa]	14.6	18.3	19.8	20.8	21.6			
$V_{\rm int,ext} [{\rm cm}^3{\rm g}^{-1}]$	0.43	0.40	0.38	0.37	0.36	0.34	0.33	0.31

Table 1S. Energetic characteristics of the {ZIF-8 + water} molecular spring

Figure 1S represents the work of intrusion and extrusion of {ZIF-8 + water} molecular spring at different temperatures and the hysteresis of their values, calculated as follows





Figure 2S represents the FTIR spectra of ZIF-8 before and after 25 cycles of intrusion-extrusion at temperatures in the range of 275 - 360K.



Figure2S. FTIR spectra of ZIF-8 before (bottom) and after (top) 25 cycles of intrusionextrusion in the 275 – 360K temperature range

Figure 3S represents the absence of visual effect of compression-decompression cycles on PVdiagrams of {ZIF-8 + water} molecular spring under different conditions.



Figure3S. 33 compression-decompression cycles of the {ZIF-8 + water} system: 2nd – 30th cycles are at 300K; 31st cycle is after keeping system at 360K and 0.1MPa during 24h; 32nd cycle is with a 24h pause at 30 MPa; 33rd cycle is at 300K after all mentioned above cycles.