SUPPORTING INFORMATION

Excess enthalpies in binary systems of isomeric C8 aliphatic monoethers with acetonitrile and their description by the COSMO-SAC model

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NMR spectra of synthesized ethers

Butyl isobutyl ether, $^{n}C_4H_9O^{i}C_4H_9$

^{1}H NMR (500 MHz, $CDCl_3$): δ/ppm=0.889 (d, 2x3H, J=6.5 Hz), 0.911 (t, 3H, J =7.5 Hz), 1.364 (m, 2H), 1.548 (m, 2H), 1.840 (m, 1H), 3.150 (d, 2H, J=7 Hz), 3.389 (t, 2H, J=7 Hz)

n-Bu-O-i-Bu

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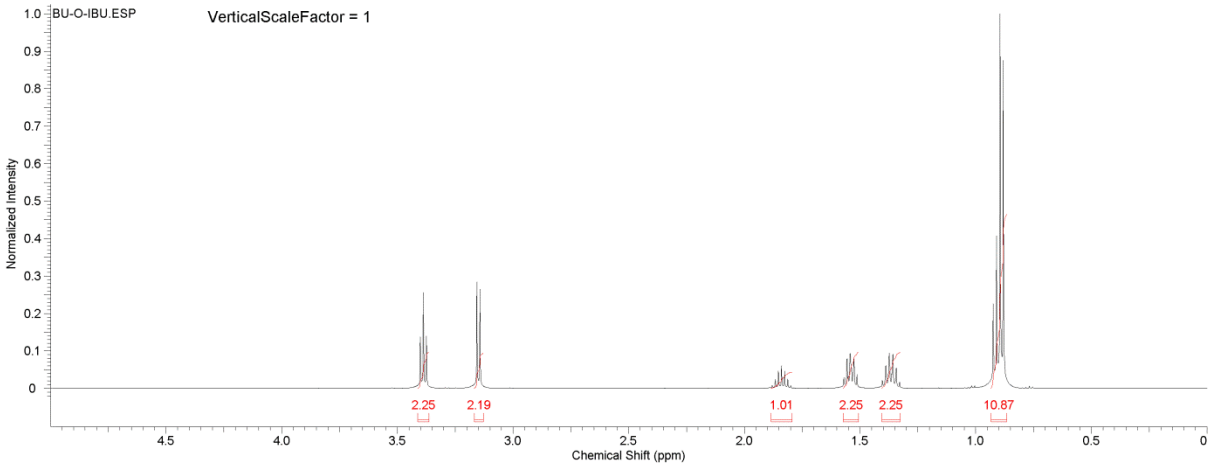
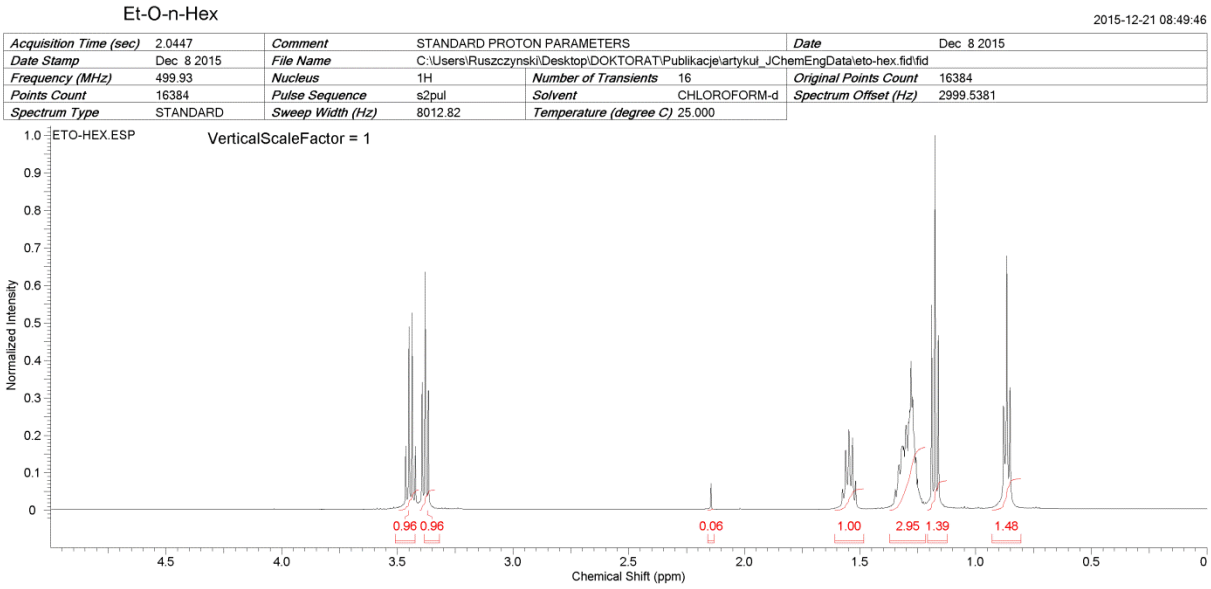
Spectrum Type	STANDARD	*Sweep Width (Hz)*	8012.82	*Temperature (degree C)*	25.000		



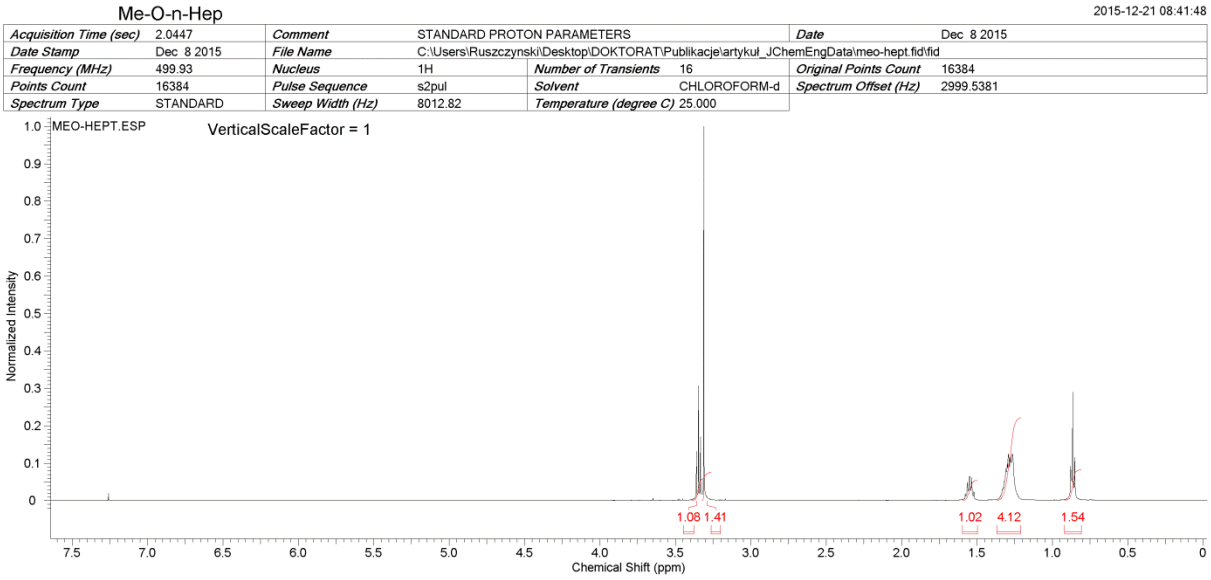
Ethyl hexyl ether, $C_2H_5O^nC_6H_{13}$

^{1}H NMR (500 MHz, $CDCl_3$): δ/ppm=0.867 (t, 3H, J=7 Hz), 1.177 (t, 3H, J=7 Hz), 1.301 (m, 6H), 1.549 (m, 2H), 3.380 (t, 2H, J=7 Hz), 3.430 (q, 2H, J=7 Hz)



Heptyl methyl ether, $CH_3O^nC_7H_{15}$

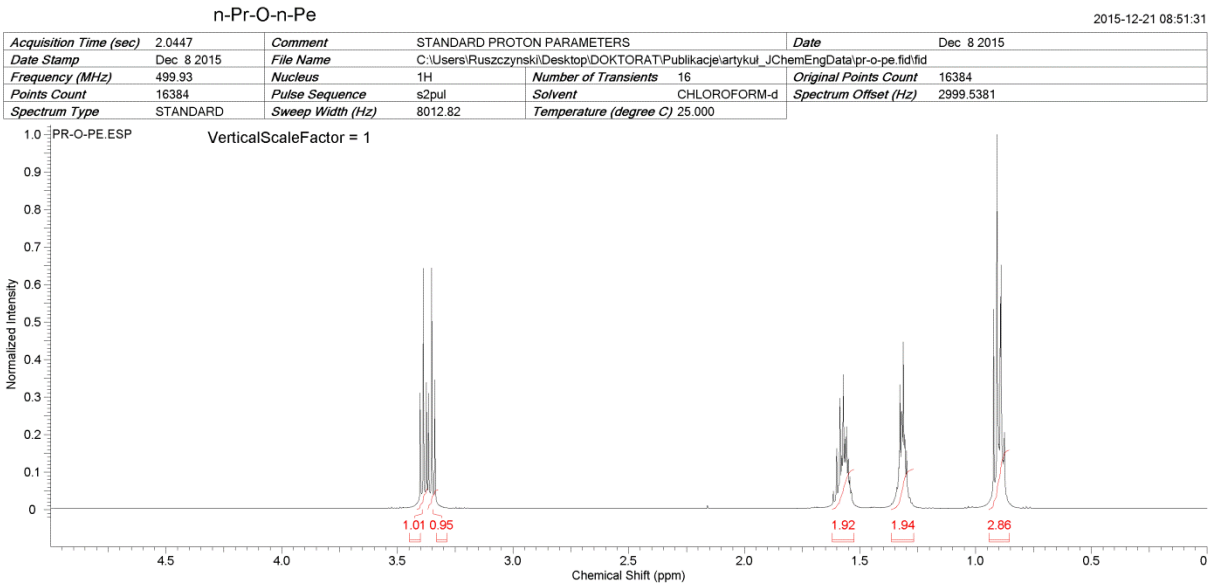
^{1}H NMR (500 MHz, $CDCl_3$): δ/ppm=0.867 (t, 3H, J=7 Hz), 1.299 (m, 8H), 1.544 (m, 2H), 3.313 (s, 3H), 3.348 (t, 2H, J =7 Hz)



Pentyl propyl ether, $^{n}C_3H_7O^{n}C_5H_{11}$

^{1}H NMR (500 MHz, $CDCl_3$): δ/ppm=0.897 (m*, 2x3H), 1.314 (m, 4H), 1.573 (m, 4H), 3.353 (t, 2H, J=7 Hz), 3.389 (t, 2H, J=7 Hz)

* two ovelapping triplets



Propyl isopentyl ether, $^{n}C_3H_7O^{i}C_5H_{11}$

^{1}H NMR (500 MHz, $CDCl_3$): δ/ppm=0.893 (d, 2x3H, J=6.5 Hz), 0.906 (t, 3H, J=7.5 Hz), 1.458 (m, 2H), 1.577(m, 2H), 1.688 (m, 1H), 3.350 (t, 2H, J=7 Hz), 3.418 (t, 2H, J=7 Hz)

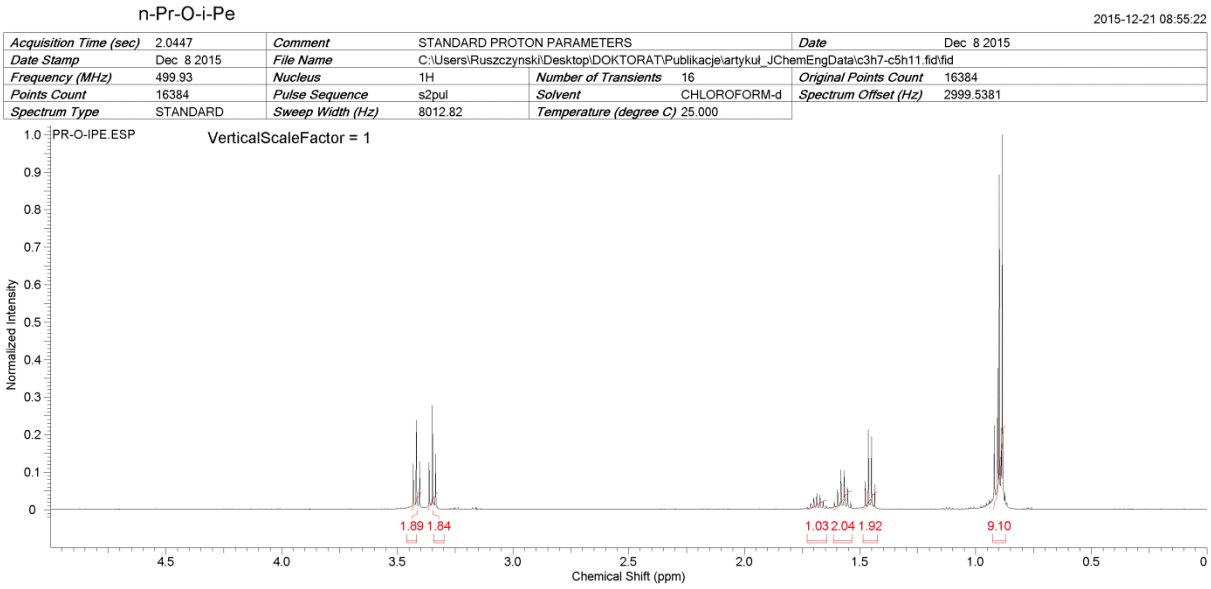


Table S1. Densities of pure C_8 ethers and acetonitrile at 0.100 MPa. The literature values are given in brackets.

T /K	$(C_4H_9)_2O$	$C_3H_7OC_5H_{11}$	$C_2H_5OC_6H_{13}$	$CH_3OC_7H_{15}$	$C_4H_9O^iC_4H_9$	$C_3H_7O^iC_5H_{11}$	CH_3CN
	ρ /g·cm^{-3}						
288.15	0.77245 (0.7725[1])	0.77345 (0.7740[1])	0.77580 (0.7777[1])	0.78389 (0.7838[1])	0.76407 (0.7640[1])	0.76879 (0.7687[1])	-
293.15	0.76805 (0.76794[3])	0.76912	0.77147	0.77971	0.75972	0.76443	-
298.15	0.76370 (0.7642[1])	0.76478 (0.7653[1])	0.76715 (0.7682[1])	0.77552 (0.7756[1])	0.75531 (0.7552[1])	0.76004 (0.7601[1])	0.77651 (0.77725[2])
303.15	0.75940 (0.75993[3])	0.76040	0.76280	0.77131	0.75087	0.75562	0.77106 (0.77183[2])
308.15	0.75500 (0.7551[1])	0.75601 (0.7560[1])	0.75845 (0.7604[1])	0.76709 (0.7670[1])	0.74645 (0.7463[1])	0.75122 (0.7512[1])	0.76559 (0.76628[2])
313.15	0.75062 (0.75144[3])	0.75160	0.75406	0.76285	0.74198	0.74678	0.76010 (0.76056[2])
318.15	0.74624	0.74719	0.74966	0.75857	0.73758	0.74231	0.75456 (0.75498[2])
323.15	0.74187 (0.74312[3])	0.74273	0.74527	0.75430	0.73299	0.73784	0.74899 (0.74919[2])

Standard uncertainties are $u(T)$ = 0.05 K, $u(p)$ = 0.005 MPa, and relative standard uncertainty $u_r(\rho)$ = 0.001.

REFERENCES

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(2) Gritsenko, N.N., Determination of polarizability and the radius of acetonitrile and dimethylacetamide molecules, *Zh. Fiz. Khim*. **1980**, *54*, 198-199.

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