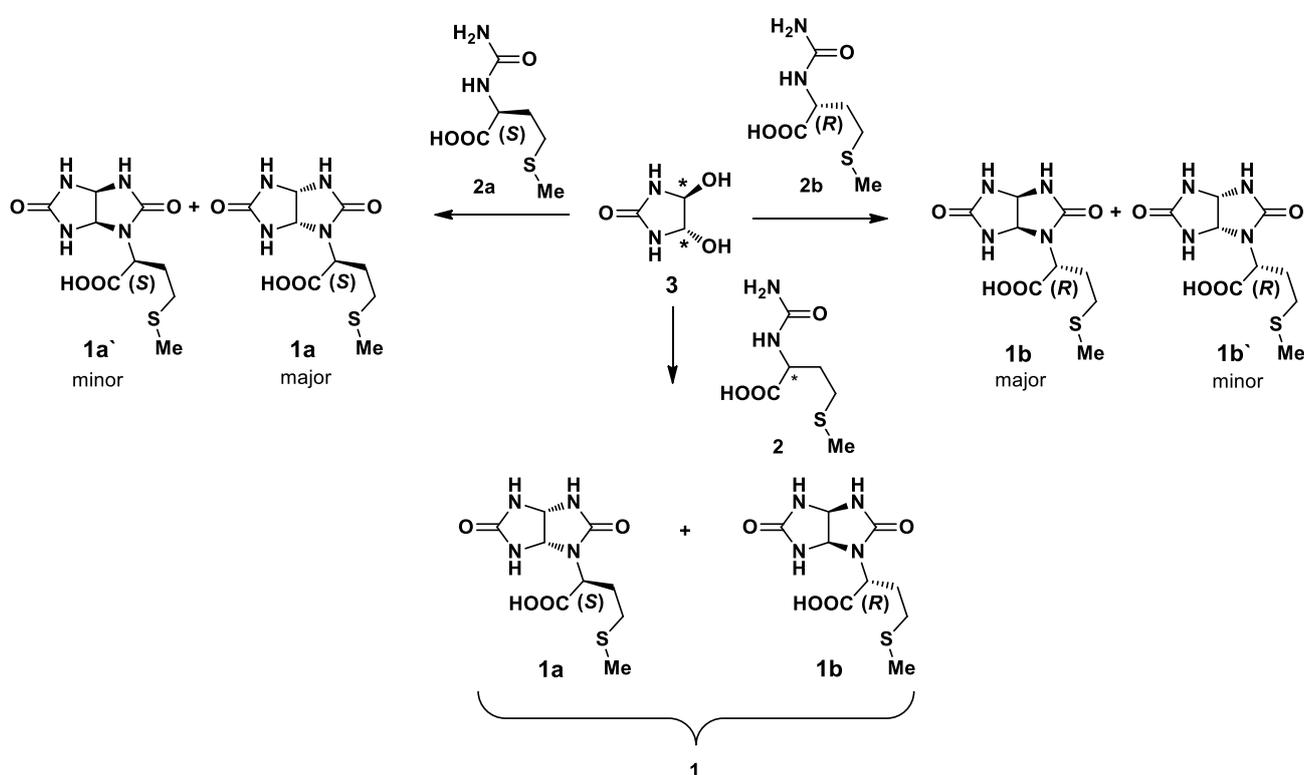


Self-organization and chirality in the high dilution solutions of glycoluril enantiomers with (*R*)- and (*S*)-methionine moieties

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Scheme S1 Diastereoselective synthesis of glycolurils **1**, **1a**, **1a'**, **1b**, **1b'**.

The physicochemical characteristics of **1a**, **1b** и **1a'**, **1b'** glycoluril stereoisomers that we isolated match the data that we published previously.^{5,11,12}

(+)-(*S*)-2-[(1*R*,5*S*)-(3,7-dioxo-2,4,6,8-tetraazabicyclo[3.3.0]oct-2-yl)]-4-methylthiobutanoic acid **1a**: mp 256-258 °C (decomp.), $[\alpha]_D^{20}$ (+)18.50 (c 2; 1N NaOH) and the ¹H and ¹³C NMR spectra match literature data.¹¹

(-)-(*S*)-2-[(1*S*,5*R*)-(3,7-dioxo-2,4,6,8-tetraazabicyclo[3.3.0]oct-2-yl)]-4-methylthiobutanoic acid **1a'**: mp 233-235 °C (decomp.), $[\alpha]_D^{20}$ (-) 77.77° (c 2; 1N NaOH) and the ¹H and ¹³C NMR spectra match literature data.¹¹

(-)-(R)-2-[(1S,5R)-(3,7-dioxo-2,4,6,8-tetraazabicyclo[3.3.0]oct-2-yl)]-4-methylthiobutanoic acid **1b**: mp 256-258 °C (decomp.), $[\alpha]_D^{20}$ (-)18.50 (c 2; 1N NaOH) and the ^1H and ^{13}C NMR spectra match literature data.¹²

(+)-(R)-2-[(1R,5S)-(3,7-dioxo-2,4,6,8-tetraazabicyclo[3.3.0]oct-2-yl)]-4-methylthiobutanoic acid **1b'**: mp 233-235 °C (decomp.), $[\alpha]_D^{20}$ (+)77.77°(c 2; 1N NaOH), and the ^1H and ^{13}C NMR spectra match literature data.⁵

Racemate 1 (1a+1b): mp 256-258 °C (decomp.), $[\alpha]_D^{20}$ 0°(c 2; 1N NaOH); the elemental analysis matches literature data.¹

Physicochemical studies

The preparation and studies of solutions were carried out using freshly prepared double distilled water with electric conductivity no higher than 1.5 $\mu\text{S}/\text{cm}$ as reported in refs. 2.

The precautions for the sample preparation include the usage of disposable pipette tips and cuvettes made of polycarbonate, disposable filters 0.45 μm (Millex HN), plastic flasks and freshly purified water. All solutions were kept sealed to prevent contaminations. For laser light scattering experiments, dust particles were removed from solution by one-time filtration using a Millipore 0.45 μm (Millex HN) filters.

The solutions were prepared by sequential tenfold dilutions from the starting concentration of $7 \times 10^{-2} \text{ mol dm}^{-3}$ of the compound. The specific electric conductivity (χ), pH, dielectric constant (ϵ) and optical activity of the solutions (α , angle of rotation of the polarization plane of light with a wavelength of sodium D-line, *i.e.* 589 nm) were measured with a inoLab Cond Level 1 conductivity meter, a BI-870 dielectric meter (Brookhaven Instruments), an “inoLab pH” pH-meter and a Perkin-Elmer-341 polarimeter using a thermally controlled cell (25 ± 0.1 °C) 0.56 dm long; the instrument accuracy was ± 0.002 degrees. The particle size (D , effective hydrodynamic diameter of kinetically mobile particles at the maximum of the distribution curve) was found by the dynamic light scattering method (DLS) using a Zetasizer Nano ZS high sensitivity analyzer (Malvern Instruments). The ζ -potential was determined by the microelectrophoresis method using the same instrument. The samples for size and ζ -potential determination were prepared in a similar way.³ All the studies were carried out at 25 °C. Experimental data were processed using standard Excel routines. The errors in the measurements of particle sizes and physicochemical properties of solutions did not exceed 15 %.

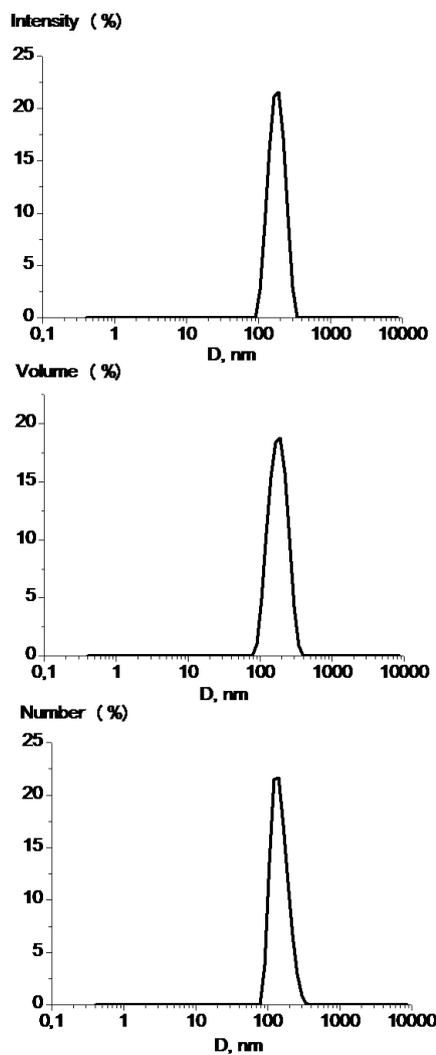


Figure S1 Particle size distribution in the aqueous solutions of compound **1a'** at $1 \times 10^{-11} \text{ mol dm}^{-3}$

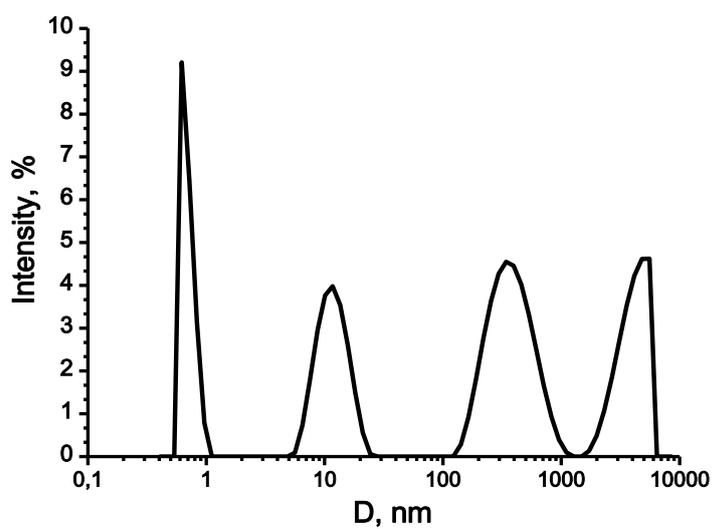


Figure S2 Particle size distribution in the aqueous solutions of compound **1b'** at $1 \times 10^{-6} \text{ mol dm}^{-3}$

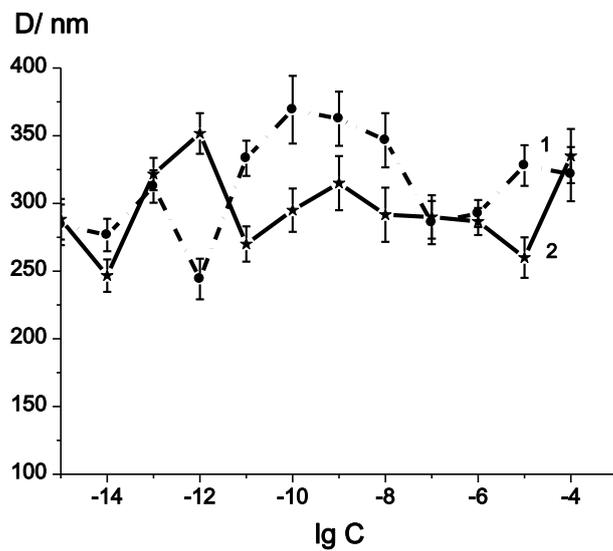


Figure S3 Plot of particle size in aqueous solutions of compounds **1a** (1) and **1a'** (2) as a function of concentration.

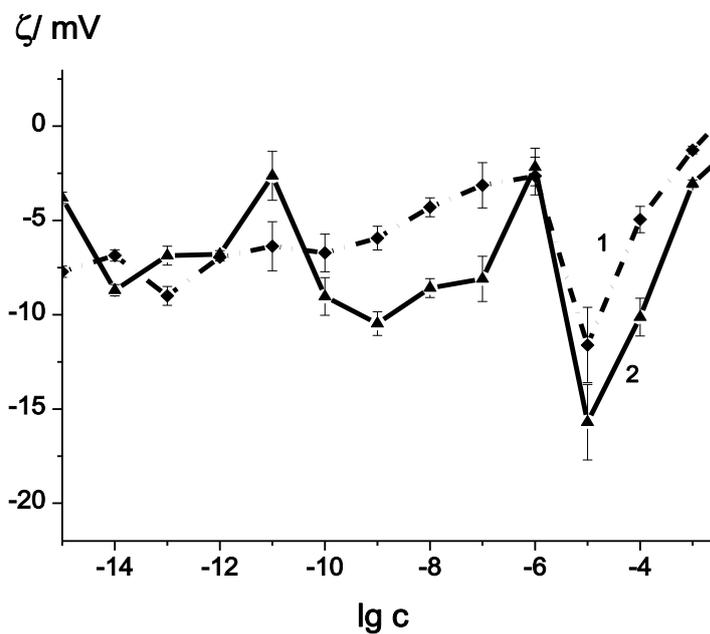


Figure S4 Plot of ζ -potential in aqueous solutions of compounds **1a** (1), **1a'** (2) versus concentration.

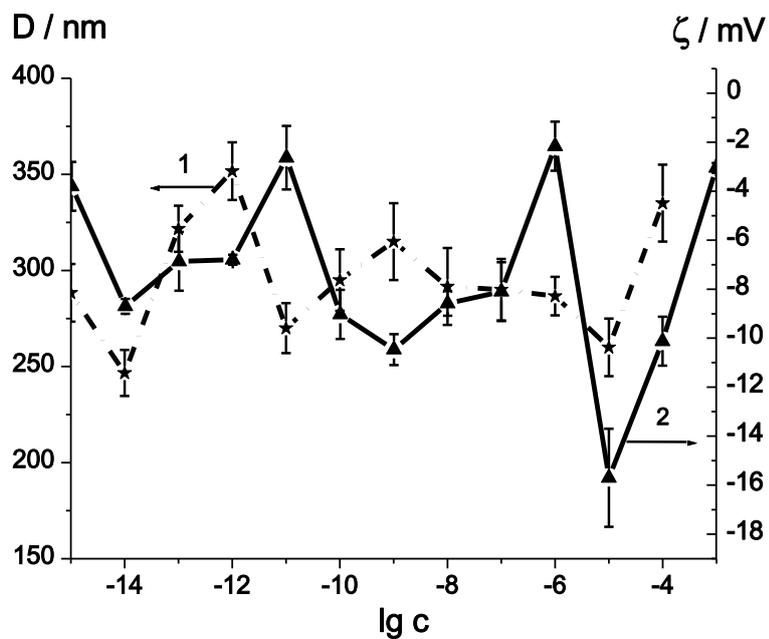


Figure S5 Plots of particle size (1) and ζ -potential (2) in aqueous solutions of compound **1a'** versus concentration.

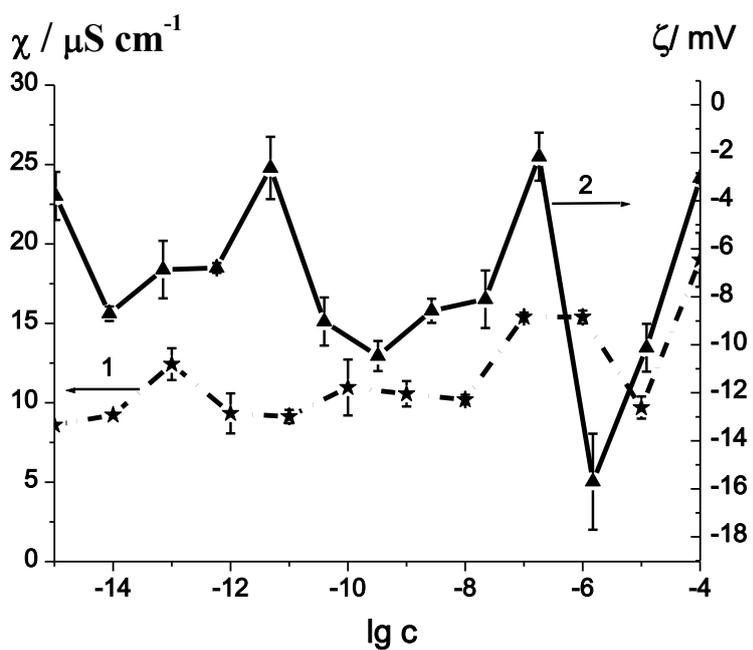


Figure S6 Plots of specific conductivity (1) and ζ -potential of particles (2) in aqueous solutions of compound **1a'** versus concentration.

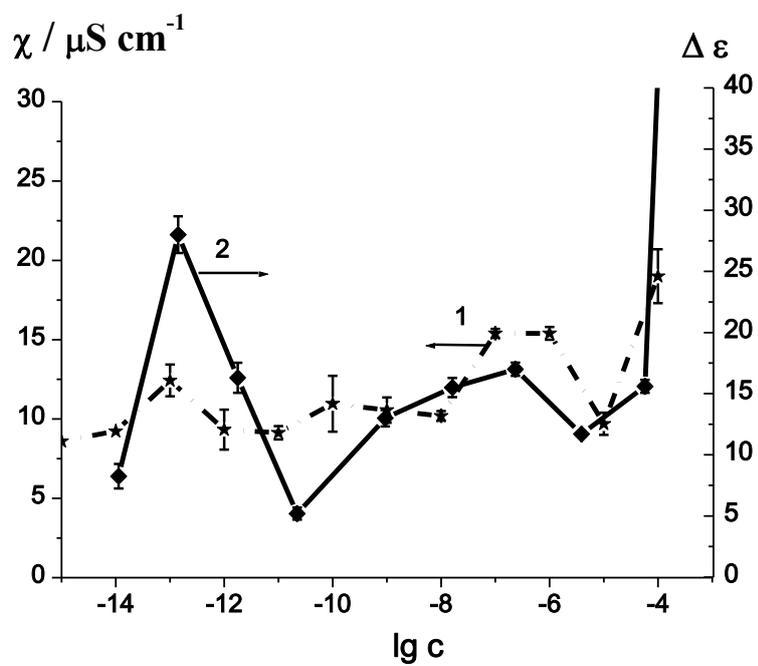


Figure S7 Plots of specific conductivity (1) and dielectric constant (2) of aqueous solutions of compound **1a'** versus concentration.

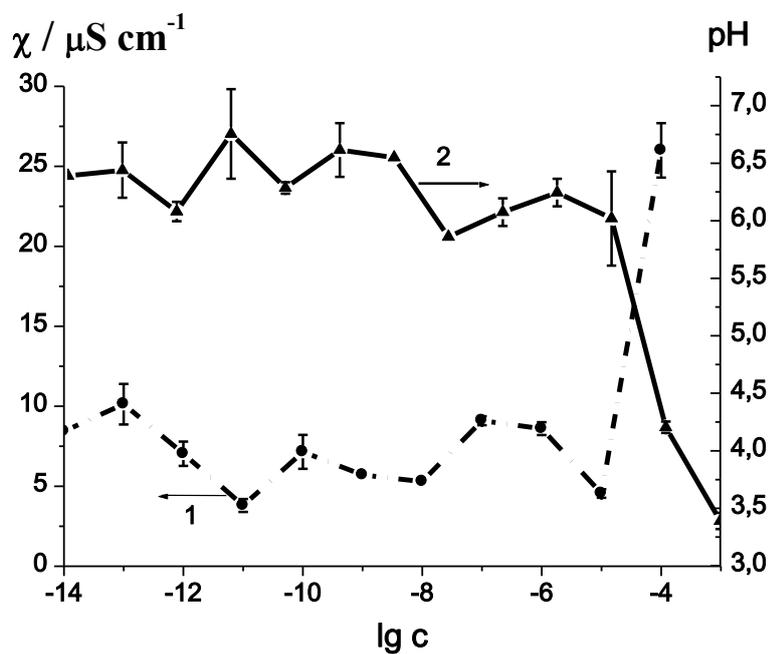


Figure S8 Plots of specific conductivity (1) and pH (2) in aqueous solutions of compound **1a'** versus concentration.

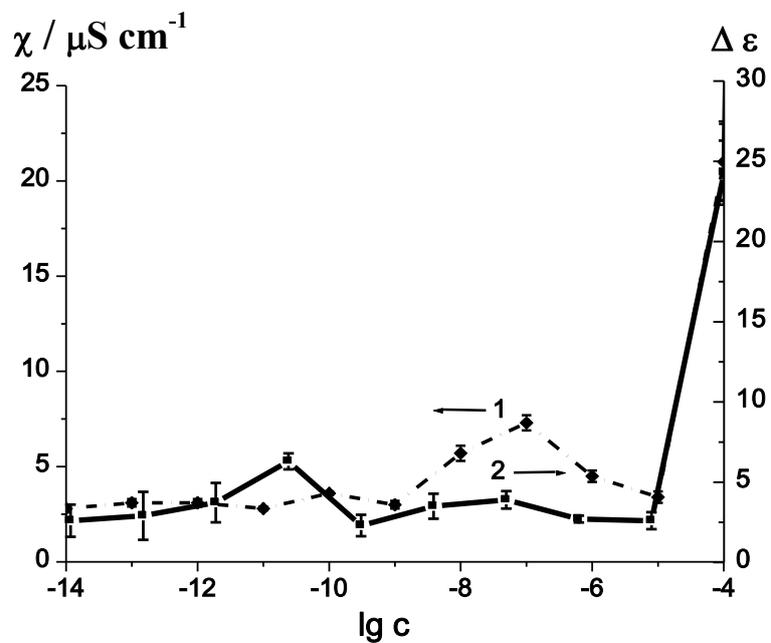


Figure S9 Plots of specific conductivity (1) and dielectric constant (2) of aqueous solutions of compound **1b'** *versus* concentration.

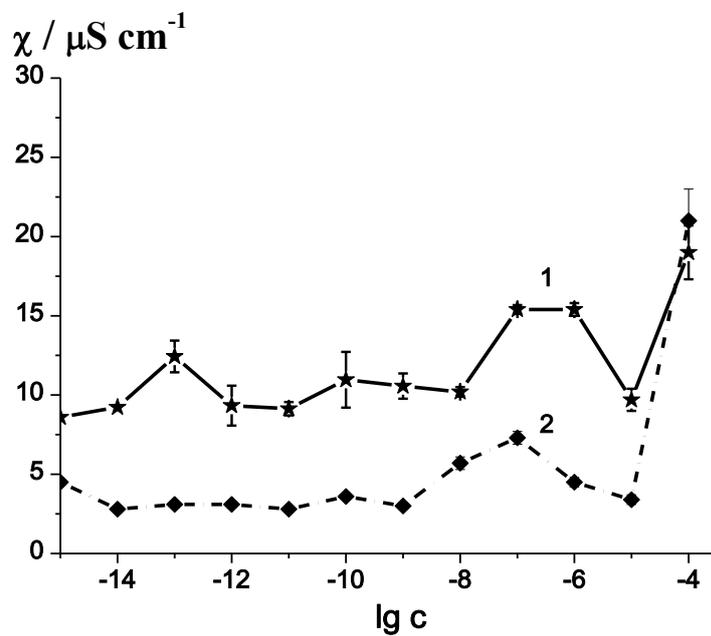


Figure S10 Plots of specific conductivity of aqueous solutions of compound **1a'** (1) and **1b'** (2) *versus* concentration.

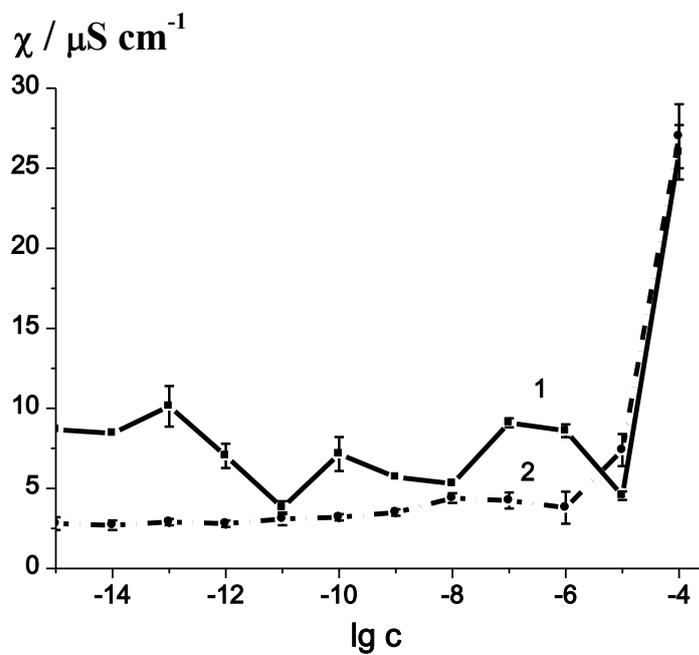


Figure S11 Plots of specific conductivity of aqueous solutions of compound **1a** (1) и **1b** (2) versus concentration.

References

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2. A. I. Konovalov and I. S. Ryzhkina, *Russ. Chem. Bull., Int. Ed.*, 2014, **63**, 1 (*Izv. Akad. Nauk, Ser. Khim.*, 2014, 1).