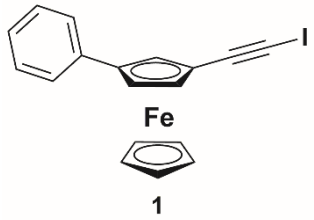
Thermodynamic study of the enantioseparation of planar chiral ferrocenes with high-performance liquid chromatography

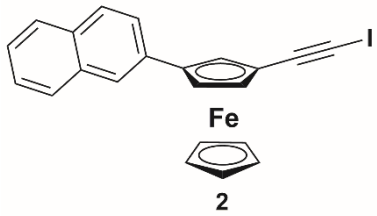
Nutsa Tsetskhladze[1], Giorgi Jibuti[1], Paola Peluso[2], Victor Mamane[3], Bezhan Chankvetadze[1]

[1]*Chair of Physical and Analytical Chemistry, Department of Chemistry, Tbilisi State University, Tbilisi, Georgia*
[2]*Istituto di Chimica Biomolecolare ICB CNR, Sede secondaria di Sassari, Sassari, Italy*
[3]*Institut de Chimie de Strasbourg, UMR 7177, CNRS-Université de Strasbourg, Strasbourg, France*
E-mail: nutsa.tsetskhladze736@ens.tsu.edu.ge

This project describes our attempt to revisit the role of temperature in the separations of enantiomers and to determine thermodynamic parameters for the enantiomers of planar chiral ferrocenes **1** and **2**[1,2] in high-performance liquid chromatography (HPLC). This can help to predict the suitable analytical conditions for the given compound in given conditions, and achieve the desired selectivity and enantiomer elution order.



1



2

For the analyzed compounds, we derived thermodynamic parameters by van't Hoff plots on an amylose-based chiral column[3] with different water ratio in acetonitrile (ACN) mobile phase (MP). Thus, the molar values of adsorption enthalpy and entropy, as well as their differences between enantiomers were calculated (see Table for the thermodynamic parameters determined for **1**). On this basis, we could evaluate if the enantioseparation was controlled by enthalpic or entropic terms and gain interesting information on the effect of adding water to the MP on both retention and selectivity.

Table. Dependence of thermodynamic parameters on water content in the MP for the enantioseparation of **1**.

water% in ACN	ΔHs (cal/mol)	ΔH_R (cal/mol)	$\Delta_{S,R}\Delta H$ (cal/mol)	ΔSs/R+lnΦ (cal/mol)	ΔS_R/R+lnΦ (cal/mol)	ΔSs/R- ΔS_R/R	T_{iso} (K)
0	-2048.6	-3525.1	-1476.5	-3.5936	-4.6729	1.0793	688.45
10	-2341.7	-3876.4	-1534.7	-3.7866	-4.5325	0.8354	1035.35
20	-2725.0	-4168.0	-1442.9	-3.5738	-4.1607	0.5869	1237.18
30	-2098.3	-3548.3	-1450.1	-1.7143	-2.3687	0.6544	1115.22
40	-1648.5	-3055.5	-1407.0	-0.2425	-0.8605	0.6180	1145.85

References

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