Spectroscopic studies of impurities on ice

Gabriela Ondrušková[1,2], Ján Krausko[1], Dominik Heger[1,2]

[1] Department of Chemistry, Faculty of Science, Masaryk University, Kamenice 5/A8, 625 00 Brno, Czech Republic

[2] Research Centre for Toxic Compounds in the Environment (RECETOX), Masaryk University, Kamenice 5/A29, 625 00 Brno, Czech Republic

Presenting author: Gabriela Ondrušková, Supervisor: Dominik Heger

The substances present in the air as pollutants may end up on ice and snow due to the processes called global distillation or grasshopper effect which involve the transport of chemical substances from warmer to colder region of the earth. These effects explain the high concentrations of the pollutants on poles. Ice and snow belong among important reaction media in which an accumulation and concentration enhancement of various types of impurities occurs. The knowledge of the location and chemical speciation of these impurities in ice and snow under various conditions is still rather limited, although crucial for the estimation of the compounds reactivity [1]. It is expected that the compounds (photo)reactivity differ depending on their particular location in/on the ice, e.g., if they are present on the surface of ice or in the spaces between ice crystals.

Therefore, we experimentally examined two scenarios that occur in the nature: freezing of solutions and deposition of the compounds from the gaseous phase. These two preparation methods yielded very contrasting results as examined by fluorescence [2]. Detailed analysis revealed distinct compounds behaviour during slow (at 253 K) and fast (at 77 K) freezing. It was observed that impurity crystals are formed at slow freezing whereas amorphous solution forms at fast freezing. Under the condition of vapor deposition to ice surface the temperature dependence was observed: at higher temperature of deposition (253 K) impurities formed crystals whereas at lower temperature of deposition (77 K) the amorphous structures formed [2].

Within our experiments, naphthalene and 1-methylnaphthalene were utilized as model compounds whose fluorescence spectroscopic properties are amply understood. At room temperature naphthalene is crystalline whereas 1-methylnaphthalene is liquid; comparison of the behaviour is currently under the scrutiny.

The results of our research have implications for the understanding of impurities in the environment as the selected substances servers as models for other compounds.

1. Yang, X.; Neděla, V.; Runštuk, J.; **Ondrušková, G.**; Krausko, J.; Vetráková, Ľ.; Heger, D. Evaporating brine from frost flowers with electron microscopy and implications for atmospheric chemistry and sea-salt aerosol formation. Atmos. Chem. Phys. 2017, 17 (10), 6291-6303.
2. **Ondrušková, G.**; Krausko, J.; Stern, J. N.; Hauptmann, A.; Loerting, T.; Heger, D. Distinct Speciation of Naphthalene Vapor Deposited on Ice Surfaces at 253 or 77 K: Formation of Submicrometer Sized Crystals or an Amorphous Layer. J. Phys. Chem. C 2018, Just Accepted Manuscript
3. Krausko, J.; Malongwe, J. K. E.; **Bičanová, G.**; Klán, P.; Nachtigallová, D.; Heger, D. Spectroscopic Properties of Naphthalene on the Surface of Ice Grains Revisited: A Combined Experimental–Computational Approach. J. Phys. Chem. A 2015, 119 (32), 8565-8578
4. Krausko, J.; **Ondrušková, G.**; Heger, D. Comment on “Photolysis of Polycyclic Aromatic Hydrocarbons on Water and Ice Surfaces” and on “Nonchromophoric Organic Matter Suppresses Polycyclic Aromatic Hydrocarbon Photolysis in Ice and at Ice Surfaces”. J. Phys. Chem. A 2015, 119 (43), 10761-10763