Tuning the adsorption potential. Separation of aromatic hydrocarbons by Cobalt and Zinc zeolitic imidazolate frameworks

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Abstract. The formation of solid solutions (alloys) is a well stablished route for tuning the functional properties in materials science, e.g. steels, semiconductors, ceramics. In porous coordination polymers, it appears as a convenient way to control the pore windows accessibility and surface properties. In this contribution, Co(II) and Zn(II) imidazoles and the mixed composition containing Zn and Co, were evaluated for aromatic hydrocarbons separation in order to illustrate the tuning of the adsorption potential through the formation of solid solutions. The best separation capability and the highest adsorption heats were observed for the mixed compositions. The random substitution of Zn by Co atoms in the network of zinc imidazolate, and vice versa, create anisotropies in the metal coordination environments, which are responsible for the appearance of local electron field gradients. This is equivalent to an increase for the adsorption potential able to interact with molecules (adsorbates) with dipole and/or quadrupole moments. Such hypothesis was corroborated for the separation of benzene, toluene and p- xylene, three molecules with quadrupole moments. The highest adsorption heat values for these adsorbates correspond to the solid containing Zn and Co. The materials under study were characterized from chemical analysis, X-ray diffraction data, thermal analysis, and specific surface measurements.

Keywords: Zeolitic Imidazolate Framework, Solid Solutions, Hydrocarbon Separation.