Mo(IV)oxophtalocyanines for Szilárd-Chalmers production of ^{99}Mo

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Emission of a prompt gamma following the reaction of a nucleus with thermal neutrons in chemical compounds can lead to breaking of chemical bonds and, therefore, ejection of the activated nucleus from the target material. This process often influences chemistry, such as oxidation state, which can be used to separate the activated nuclei. [1]

This so called Szilárd-Chalmers (S-C) Reactions is especially interesting for medical applications since neutron capture by ^{98}Mo (natural abundance: 24.4 %) yields ^{99}Mo, which in turn by decay, yields medically important ^{99m}Tc.

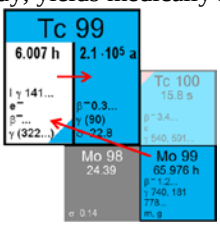

Figure 1: *Production and decay scheme of ^{99m}Tc [2]*

One main dimension to characterize S-C reactions is the retention – the amount of activity that remains in the target molecule after the separation of the radionucleus.

A small retention means little bond reformation. Bond reformation can be influenced by the chemical environment including substituents on the parent molecule among other factors.

Experimental

Molybdenum(IV)oxophthalocyanines (MoO(XPc))were chosen as target materials, as they are thermally and chemically very stable [3] and therefore well-suited to study the influence of substituents on S-C reactions.

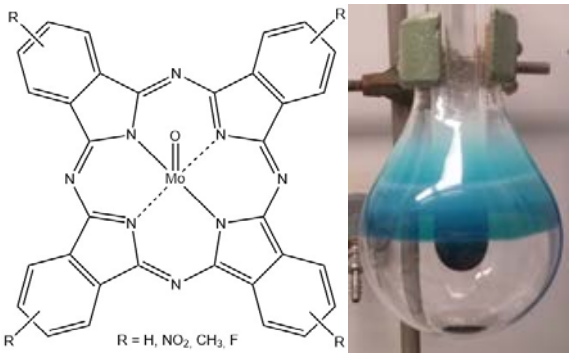

Figure 1: *left: structure of MoO(XPc); right: characteristic blue colour of MoO(CH$_3$Pc)*

Three substituents (X) with different electronic behavior were synthesized, purified and characterized: nitro (-NO2), methyl (-CH3) and fluoro (-F) (Figure 1).

Experiments were carried out in dry irradiation tubes at the edge of the TRIGA mark II research reactor at the TU Wien (irradiation time: 1 h, neutron flux: $2 \cdot 10^{12}$ cm^{-2}s^{-1}). After separation of the ^{99}Mo from the target material with ammonia (25%, 5 mL) the determination of the retention was carried out with gammaspectroscopy using the 180 keV line of ^{99}Mo.

Results & Outlook

Calculation of the retention shows a very good result for (4) with retention of 3.3%, (1) and (2) show moderate retention with 13.5% and 10.0%, respectively and only (2) show an excessive retention with almost 30% retention (Figure 2).

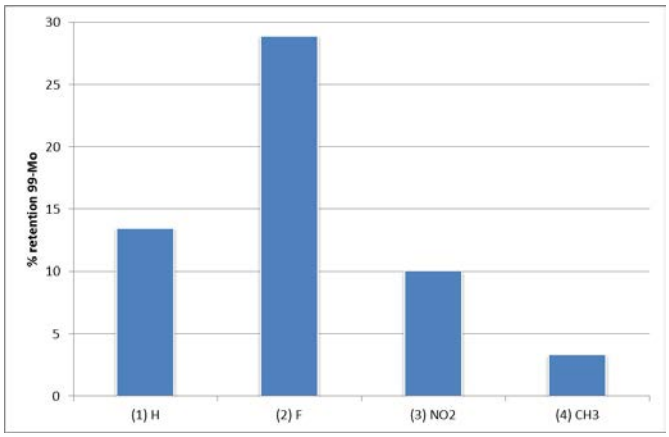

Figure 2: Retention of ^{99}Mo for all target materials.

The high retention of (2) may be explained with the reactivity of the fluoride substituent which can lead to more recombination reactions and therefore to a higher retention.

The low retention and quite good yield, as well the relatively easy purification of MoO(CH3Pc) makes it a good starting point for further investigations.

[1] H. Müller, H. Hot Atom Chemistry in Inorganic Solids — The Present Status and Future Aspects. Radiochim. Acta 28, **1981**.
[2] Extract from the *Karlsruhe Nuclide Chart*, 8th Edition, **2012**.
[3] N.B. McKeown, *Science of Synthesis, Product Class 9: Phthalocyanines and Related Compounds*.