PBT assessment of Balsams, copaiba, sulfurised, mixed with turpentine, gold salts

1 Initial approach

Balsams, copaiba, sulfurised, mixed with turpentine, gold salts is a UVCB substance and its composition is not well defined. The substance is being registered at 1 – 10 tpa and therefore an assessment of Annex III derogations is required. It has been confirmed that the substance has no widespread or dispersive uses and it is not considered to be CMR based on a lack of published information. A PBT assessment is required before the Annex III assessment can be finalised. In order to conduct this, a partition coefficient test was commissioned at Harlan Laboratories. Initial draft results from this study, received from Harlan Laboratories on 20 February 2012, indicated that a partition coefficient could not be measured due to the low solubility of the test item. On this basis a recommendation was made in the draft Updated ITS report[1], issued to the PMC on 29 February 2012, to conduct a ready biodegradation study. As no partition coefficient could be measured, and insufficient structural information is available for this substance to determine a Kow value using QSARs, it seemed appropriate to conduct a biodegradation study to either confirm that the substance is not PBT, or to fill an Annex VII endpoint if it is determined that Annex III exemptions do not apply.

2 Proposed changes to the approach

Following the completion of the draft Updated ITS report, Harlan issued the full draft report on the physico-chemical properties of Balsams, copaiba, sulfurised, mixed with turpentine, gold salts. After reviewing the report from Harlan, it emerged that some solubility data are available that could be used to estimate the partition coefficient of the substance. Further discussion with Harlan determined that it is definitely not possible to conduct further testing as very little compositional information is available. In the water solubility test the organic component was measured as Total Organic Carbon (TOC) in the filtered supernatant, but this could not be used in a partition coefficient study because of interference from the octanol, even in the aqueous phase (as this is saturated with octanol prior to the test). The only way a partition coefficient could potentially be determined would be by monitoring the gold component of the substance. However, it is the organic component and not the metallic component that is considered to be most relevant for assessing the bioaccumulation potential of an organometallic substance. Analysing the gold component would not, therefore, be likely to provide any additional useful information about the bioaccumulation potential of the substance. Estimation of a partition coefficient value based on the solubility data already included in the report could still be an option, however.

[1] Gold_Phase III_Updated ITS_20120228

3 Partition coefficient estimation

3.1 Solubility data

The solubility data that are available from the Harlan test report are as follows:

Water solubility

As this is an organometallic substance water solubility was determined by measuring gold and Total Organic Carbon (TOC). Water solubility results based on gold and based on TOC are presented below.

Measuring the gold concentration: $<1.0 \times 10^{-5}$ g L^{-1} at 20°C, equivalent to a concentration of Balsams, copaiba, sulfurised, mixed with turpentine, gold salts of $<1.9 \times 10^{-5}$ g L^{-1}

Measuring mean dissolved TOC: 5.28×10^{-3} g L^{-1} at 20°C

Solubility in octanol

Solubility in octanol was determined based on visual assessment, as follows:

$< 9 \times 10^{-3}$ g L^{-1}, shaking at an elevated temperature of 30°C for 21 hours

3.2 Substance composition

Little compositional information is available for this substance therefore some assumptions have had to be made.

The gold content of the substance is known to be 53%. The organic content of the substance is therefore 47%. Assuming that the organic component is an alkane (empirical formula C_NH_{2N+2}) the carbon content of the organic component would be approximately 85%. This would make the carbon content of the substance equal to approximately 40%.

3.3 Calculating the partition coefficient

If the carbon content of the substance is assumed to be 40%, the solubility of the substance in water can be determined based on the mean dissolved TOC measurement and the percentage carbon content of the substance, as below:

5.28 mg L^{-1} / 0.4 = 13.2 mg L^{-1}

The solubility of the substance in octanol (determined by visual assessment) was stated in the Harlan report, as below:

<9 mg L^{-1}

The octanol water partition coefficient can be estimated for the substance by assuming that the identified limit of solubility would be achieved in each phase during a test. The partition

coefficient is therefore calculated as the solubility in octanol divided by the solubility in water, i.e.

K_{OW} = 9 / 13.2 = 0.68

Log K_{OW} = $\log_{10}$(0.68) = -0.17.

3.4 Alternative assumptions

This estimate of the log K_{OW} value of the substance may be an overestimation as the water solubility is known (although the carbon content of the substance is not precisely known), whereas the octanol solubility is a maximum limit value. A lower solubility in octanol would result in a lower log K_{OW} value for the substance. Overestimation of the carbon content of the substance would lead to an underestimation of the water solubility, which would result in overestimation of the octanol water partition coefficient. Underestimation of the C content of the substance would result in an underestimation of the partition coefficient. Assuming that the C content of the substance is 47% (i.e. the maximum possible proportion based on the gold content of the substance) results in an estimated log K_{OW} value of -0.1.

If the water solubility of the substance, as calculated from the gold concentration, was used as the water solubility estimate for calculation of the octanol water partition coefficient the resulting log K_{OW} value would be 2.68. This is likely to considerably overestimate the true octanol water partition coefficient of the organic component of the substance, because the solubility based on TOC analysis was considerably higher. This high estimate of the log K_{OW} value for the substance is still appreciably below the threshold for identification of substances as potentially bioaccumulative.

4 Recommendations

As the estimated partition coefficient is several orders of magnitude below the threshold for Bioaccumulation (log K_{OW} 4.5) it is extremely unlikely that the substance is bioaccumulative, and should therefore not be classified as PBT. It is recommended that the estimated K_{OW} value is used for the PBT assessment of this substance, rather than conducting a biodegradation study. Conducting a biodegradation test for this substance would be very challenging due to the low test item solubility and lack of compositional data for the test substance. As the estimated partition coefficient value is so low it would seem appropriate to use this reasoning as justification for identifying the substance as not PBT, rather than to attempt a biodegradation study on a difficult substance such as this. However, if ECHA do not accept this approach then a biodegradation study may need to be conducted at a later stage.