

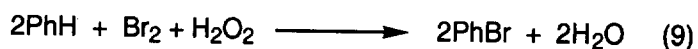
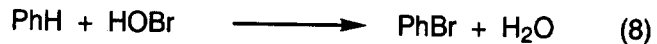
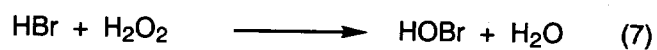
**Supporting information for:**

**Vanadium-catalysed oxidative bromination using dilute mineral acids and hydrogen peroxide: an option for recycling waste acid streams / Gadi Rothenberg and James H. Clark.**

As a basis for comparison, it is taken that bromination occurs either using  $\text{Br}_2$  (when present) or  $\text{HOBr}$ . The interconversions  $\text{HOBr} + \text{HBr} \rightleftharpoons \text{Br}_2 + \text{H}_2\text{O}$ , and  $\text{Br}_2 + \text{Br}^- \rightleftharpoons \text{Br}_3^-$ , are disregarded. The calculation of E-factors is based on the theoretical conversion of  $\text{PhH}$  to  $\text{PhBr}$  (assuming 100% yield).

Example (1). For the reaction  $\text{PhH} + \text{Br}_2 \Rightarrow \text{PhBr} + \text{HBr}$ , 80.9 g  $\text{HBr}$  (waste) for every 156.9 g  $\text{PhBr}$  (product) is produced, ergo  $E=80.9/156.9 = 0.51$ .

Example (2). When using  $\text{Br}_2 + \text{H}_2\text{O}_2$ , the reactions are:



Resulting in 36 g  $\text{H}_2\text{O}$  (waste) for every 313.8 g  $\text{PhBr}$  (product), ergo  $E=36/313.8 = 0.11$ .