Synthesis of barium peroxide - Protocol A

$$BaCl_2 + H_2O_2 + 8H_2O \rightarrow BaO_2.8H_2O + 2HCl$$

Reaction. In a flask, dissolve about 5 g (24.01 mmol) of barium chloride in 200 mL of distilled water. In a beaker, place 15 mL of 25% solution of ammonium hydroxide, 30 mL (53.57 mmol) of hydrogen peroxide solution 20 vol (about 123% excess) and cool in ice. Fit a funnel and add, dropwise and with stirring, the barium chloride solution. When the addition is complete, maintain the reaction mixture in ice for 20 to 30 minutes.

Isolation. Filter the crystals by suction, wash with cold distilled water, ethanol and ethyl ether and air dry.

Purification. Not prescribed.

Safety. See hazards associated with the reagents in Table 1.

Greenness Assessment. The evaluation was performed using the Green Star (GS) and the results are shown in Figure 1.

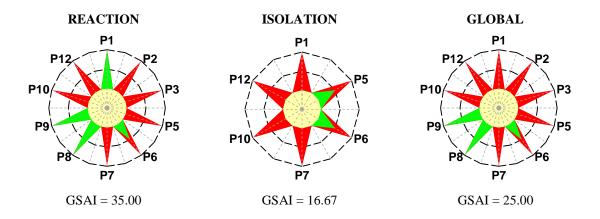


Figure 1. Greenness assessment (GS) for the synthesis of barium peroxide

Construction of the GS

 $BaCl_2 + H_2O_2 + 8H_2O \rightarrow BaO_2.8H_2O + 2HCl$

Table 1 presents the hazards and scores associated with the substances involved and Table 2 presents the scores used to construct the green stars.

Table 1. Hazards for the synthesis of barium peroxide, protocol A^{α}

Substances involved	Step			Hazard code	Score: hazards to		
Substances involved	R I		Pu	Tiazara code	НН	E	P
Stoichiometric reagents							
Barium chloride (CAS 10361-37-2)	✓			H301, H332	3	1	1
Hydrogen peroxide (solution)	✓			H302, H318	3	1	1
Auxiliary substances							
Solvents							
Ammonium hydroxide (25% solution)	✓			H290, H314, H335, H400	3	3	2
Ethanol ^b (CAS 64-17-5)		✓		H225	1	1	3
Ethyl ether (CAS 60-29-7)		✓		H224, H302, H336, EUH019, EUH066	2	1	3
Water ^{a,b}	✓	✓		-	1	1	1
Product							
Barium peroxide (1304-29-6)	✓	✓		H272 (cat. 2), H302, H332	2	1	3
Waste							
Ammonium hydroxide (dilute solution)		✓		H315, H318, H400	3	3	1
Ethanol ^b		✓		H225	1	1	3
Ethyl ether		✓		H224, H302, H336, EUH019, EUH066	2	1	3
Hydrochloric acid (dilute solution)		✓		-	1	1	1
Hydrogen peroxide (dilute solution)		✓		-	1	1	1
Water ^{a,b}		✓		-	1	1	1

α R – Reaction; I – Isolation; Pu – Purification; HH – Human Health; E – Environment; P – Physical

^a Renewable; ^b Degradable to innocuous products

Table 2. Scores used to construct the green star for the synthesis of barium peroxide, protocol A^{α}

Green Chemistry	Reaction			Isolation	Global		
Principle		Explanation		s Explanation		Explanation	
P1 Prevention	3	Without waste	1	Dilute ammonium hydroxide, H318 and H400	1	Dilute ammonium hydroxide, H318 and H400	
P2 Atom Economy	1	Excess of hydrogen peroxide > 10%, formation of by- products		NA	1	Excess of hydrogen peroxide > 10%, formation of by-products	
P3 Less hazardous chemical synthesis	1	Barium chloride, H301, hydrogen peroxide, H318, and ammonium hydroxide, H314 and H400		NA	1	Barium chloride, H301, hydrogen peroxide, H318, and ammonium hydroxide, H314 and H400	
P5 Safer solvents and auxiliary substances	1	Ammonium hydroxide, H314 and H400		Ethyl ether, H302, H336 and EUH066	1	Ammonium hydroxide, H314 and H400	
P6 Increase energy efficiency	2	$0 ^{\circ}\text{C} \le \text{T} \le 100 ^{\circ}\text{C}$	2	$0 {}^{\circ}\text{C} \le \text{T} \le 100 {}^{\circ}\text{C}$	2	$0 {}^{\circ}\text{C} \le \text{T} \le 100 {}^{\circ}\text{C}$	
P7 Use renewable feedstocks	1	Substances not renewable		Substances not renewable	1	Substances not renewable	
P8 Reduce derivatives	3	One stage		NA	3	One stage	
P9 Catalysts	3	Without catalysts		NA	3	Without catalysts	
P10 Design for degradation	1	Substances not degradable	1	Substances not degradable	1	Substances not degradable	
P12 Safer chemistry for accident prevention	1	Barium chloride, H301, hydrogen peroxide, H318, ammonium hydroxide, H314, and barium peroxide, H272 (cat.2)		Ethanol, H225, ethyl ether, H224, barium peroxide, H272 (cat.2), and ammonium hydroxide, H314	1	Barium chloride, H301, hydrogen peroxide, H318, ammonium hydroxide, H314, barium peroxide, H272 (cat.2), ethanol, H225, and ethyl ether, H224	

 $^{^{\}alpha}s$ – Score; NA – Not applicable

References

Instituto Superior Técnico – Universidade Técnica de Lisboa, https://fenix.ist.utl.pt/disciplinas/lq-i/2010-2011/1-semestre (accessed February 2011).