# Synthesis of barium peroxide – Protocol B

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

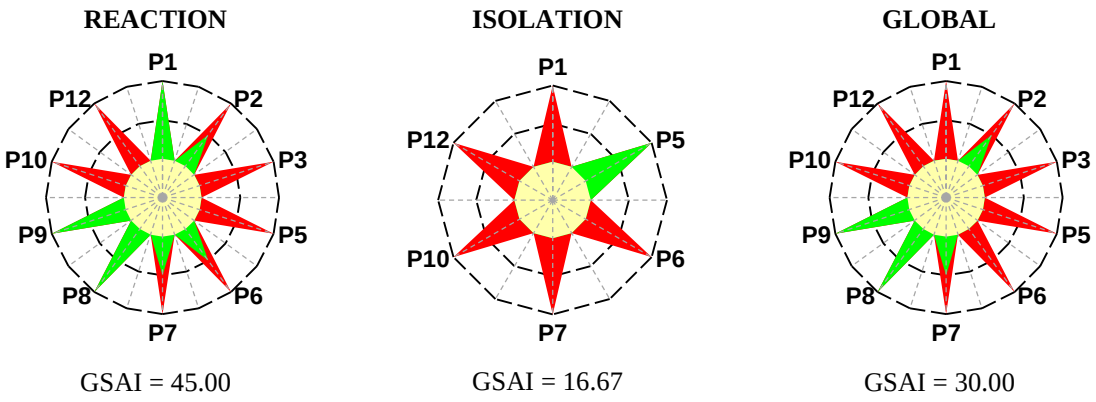
**Reaction.** Under a nitrogen atmosphere, add a solution of hydrogen peroxide (stoichiometric proportions) and a solution of ammonium hydroxide to an aqueous solution of barium chloride. Place the mixture in an ice bath to precipitate the product.

**Isolation.** Collect by filtration the barium peroxide precipitated and dry at 150 ºC.

**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.




GSAI = 45.00 GSAI = 16.67 GSAI = 30.00

**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 B[α]

| Substances involved | Step | | | Hazard code | Score: hazards to... | | |
|---|---|---|---|---|---|---|---|
| | R | I | Pu | | HH | E | P |
| **Reagentes estequiométricos** | | | | | | | |
| Barium chloride (CAS 10361-37-2) | ✓ | | | H301, H332 | 3 | 1 | 1 |
| Hydrogen peroxide (CAS 7722-84-1) | ✓ | | | H302, H318 | 3 | 1 | 1 |
| **Auxiliary substances** | | | | | | | |
| **Solvents** | | | | | | | |
| Ammonium hydroxide (solution) | ✓ | | | H290, H314, H335, H400 | 3 | 3 | 2 |
| Water[a,b] | ✓ | | | - | 1 | 1 | 1 |
| **Other auxiliary substances** | | | | | | | |
| Nitrogen[a] (CAS 7727-37-9) | ✓ | | | H280 | 1 | 1 | 2 |
| **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 |
| Hydrochloric acid (dilute solution) | | ✓ | | - | 1 | 1 | 1 |
| Nitrogen[a] | ✓ | | | H280 | 1 | 1 | 2 |
| 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 B[α]

| Green Chemistry Principle | Reaction | | Isolation | | Global | |
|---|---|---|---|---|---|---|
| | **s** | **Explanation** | **s** | **Explanation** | **s** | **Explanation** |
| **P1** Prevention | 3 | Nitrogen | 1 | Dilute ammonium hydroxide, H318 and H400 | 1 | Dilute ammonium hydroxide, H318 and H400 |
| **P2** Atom Economy | 2 | Stoichiometric proportions of reagents, formation of by-products | | NA | 2 | Stoichiometric proportions of reagents, 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 | 3 | Solvents and auxiliary substances are not used | 1 | Ammonium hydroxide, H314 and H400 |
| **P6** Increase energy efficiency | 2 | 0 ºC ≤ T ≤ 100 ºC | 1 | T > 100 ºC | 1 | T > 100 ºC |
| **P7** Use renewable feedstocks | 2 | Nitrogen is renewable | 1 | Substances not renewable | 2 | Nitrogen is 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) | 1 | Barium peroxide, H272 (cat.2), and ammonium hydroxide, H314 | 1 | Barium chloride, H301, hydrogen peroxide, H318, ammonium hydroxide, H314, and barium peroxide, H272 (cat.2) |

[α]s – Score; NA – Not applicable

## References

Kopnin, E.M. *et al*. New Family of Au-Based Superconductors $AuBa_2Ca_{n-1}Cu_nO_{2n+3}$ (n = 3,4). *Chem. Mater*., **2001**, *13*, 2905-2908.