**Electronic supplementary information for**

**Biomolecule-assisted route to obtain nanostructured bismuth oxybromide with enhanced photocatalytic activity**

Genesis de O. Limaa, Thaylan P. Araújoa, José Renato de O. Limab, Gilza Maria P. Prazeresa, Carlos William A. Paschoalc, Elson Longod, Auro A. Tanakaa, Adeilton P. Maciela, Diego A. B. Barbosae, Marcio Aurélio P. Almeidab\*

\*Corresponding author.

E-mail address: almeida.marcio@ufma.br (Marcio Almeida).

|  |  |
| --- | --- |
| C:\Users\BCT\Documents\Orientações\Genesis\Imagens\Gly\BBrGL__009.tif  **(a)** | C:\Users\BCT\Documents\Orientações\Genesis\Imagens\Gly\BBrGL__011.tif  **190 nm**  **(b)** |
| C:\Users\BCT\Documents\Orientações\Genesis\Imagens\Gly\BBrGL__008.tif  **5.8 μm**  **5.3 μm**  **(c)** | C:\Users\BCT\Documents\Orientações\Genesis\Imagens\Phe\BBrRhe__010.tif  **(d)** |

Fig. S1 FEG-SEM images of the as-prepared samples. *a, b, c)* BOB-gly. *c)* BOB-phe.

|  |
| --- |
| C:\Users\Marcio Almeida\Documents\Papers_2019\Genesis\BET\Fig. S3.jpg |

Fig. S3 Nitrogen adsorption–desorption isotherms of the BiOBr compounds.

Table S1.Refined structural data for the BiOBr samples, based on tetragonal symmetry.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Space group: *P4/nmm* (#129); Z=2 | | | | | | | | |
| BOB | | | | | | | | |
| Cell parameters: a=3.91716(15) Å; c=8.08797(33) Å; cell volume 124.10(1) Å3 | | | | | | | | |
| Fractional coordinates | | | | | | | | |
| Label | Wyckoff site | x | y | | z | | Occ. | Uiso |
| Bi1 | 8j | 0.25 | 0.25 | | 0.15389(16) | | 1 | 0.02876(35) |
| Br1 | 8j | 0.25 | 0.75 | | 0.65743(40) | | 1 | 0.03449(101) |
| O1 | 4d | 0.25 | 0.75 | | 0 | | 1 | 0.025 |
| Bismuth bond angles | | | | | | | | |
| Atom 1 | Atom 2 | Distance 1,2 (Å) | | Atom 3 | Distance 1,3 (Å) | | Bond angle (°) |  |
| Bi | Br | 3.1698(17) | | O | 2.3251(8) | | 74.786(41) |  |
|  | Br | 3.1698(17) | | Br | 3.1698(17) | | 76.465(51) |  |
|  | O | 2.3251(8) | | O | 2.3251(8) | | 73.251(25) |  |
| Bonds | | | | | | | | |
| Atom 1 | Atom 2 |  | Bond distance (Å) | | |  |  |  |
| Bi | Br | 4x | 3.1698(17) | | |  |  |  |
|  | O1 | 4x | 2.3251(8) | | |  |  |  |
| BOB-phe | | | | | | | | |
| Cell parameters: a=3.91937(48) Å; c=8.09242(116) Å; cell volume 124.31(3) Å3 | | | | | | | | |
| Fractional coordinates | | | | | | | | |
| Label | Wyckoff site | x | y | | z | | Occ. | Uiso |
| Bi1 | 8j | 0.25 | 0.25 | | 0.15218(18) | | 1 | 0.03946(54) |
| Br1 | 8j | 0.25 | 0.75 | | 0.65919(43) | | 1 | 0.04905(167) |
| O1 | 4d | 0.25 | 0.75 | | 0 | | 1 | 0.025 |
| Bismuth bond angles | | | | | | | | |
| Atom 1 | Atom 2 | Distance 1,2 (Å) | | Atom 3 | Distance 1,3 (Å) | | Bond angle (°) |  |
| Bi | Br | 3.1676(17) | | O | 2.3173(8) | | 74.492(41) |  |
|  | Br | 3.1676(17) | | Br | 3.1676(17) | | 76.531(51) |  |
|  | O | 2.3173(8) | | O | 2.3225 (9) | | 73.539(25) |  |
| Bonds | | | | | | | | |
| Atom 1 | Atom 2 |  | Bond distance (Å) | | |  |  |  |
| Bi | Br | 4x | 3.1676(17) | | |  |  |  |
|  | O1 | 4x | 2.3173(8) | | |  |  |  |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Space Group: P4/nmm (#129); Z=2** | | | | | | | | | |
| **BOB-gly** | | | | | | | | | |
| Cell parameters: a=3.91936(15) Å, c=8.09196(32) Å; Cell volume 124.30(1) Å3 | | | | | | | | | |
| Fractional Coordinates | | | | | | | | | |
| Label | Wyckoff Site | x | y | | z | | Occ. | Uiso | |
| Bi1 | 8j | 0.25 | 0.25 | | 0.15340(15) | | 1 | 0.02908(30) | |
| Br1 | 8j | 0.25 | 0.75 | | 0.65951(38) | | 1 | 0.03492(87) | |
| O1 | 4d | 0.25 | 0.75 | | 0 | | 1 | 0.025 | |
| Bismuth Bond Angles | | | | | | | | | |
| Atom 1 | Atom 2 | Distance 1.2 (Å) | | Atom 3 | Distance 1.3 (Å) | | Bond Angle (°) | |  |
| Bi | Br | 3.1680(17) | | O | 2.3248(7) | | 74.723(39) | |  |
|  | Br | 3.1680(17) | | Br | 3.1680(17) | | 76.522(51) | |  |
|  | O | 2.3248(7) | | O | 2.3248(7) | | 73.265(22) | |  |
| Bonds | | | | | | | | | |
| Atom 1 | Atom 2 |  | Bond Distance (Å) | | |  |  | |  |
| Bi | Br | 4x | 3.1680(17) | | |  |  | |  |
|  | O1 | 4x | 2.3248(7) | | |  |  | |  |

Table S2.Refined structural data for samples BOB-gly in the basis of the tetragonal symmetry

Table S3.Parameters of nitrogen adsorption–desorption isotherms of the BiOBr compounds

|  |  |  |  |
| --- | --- | --- | --- |
| **Parameter** | **BOB** | **BOB-gly** | **BOB-phe** |
| Correlation Coefficient | 0.9999078 | 0.9995173 | 0.9998873 |
| Specific area, SBET (m2/g) | 2.0217 | 7.6950 | 6.3410 |
| Total pore volume, VBJH (cm3/g) | 0.006697 | 0.038963 | 0.026159 |
| Pore diameter, Dp (Å)\* | 129.435 | 161.975 | 147.092 |

\* BJH Desorption average pore diameter.