TABLE I. Blank experiments on catalytic oxidation of styrene

|  |  |  |  |
| --- | --- | --- | --- |
| **Entry** | **Catalyst** | **Oxidant** | **Conversion, %** |
| 1 | none | TBHP | 0 |
| 2 | none | H2O2 | 0 |
| 3 | **1** | none | 0 |
| 4 | **3** | none | a0 |
| 5 | **5** | none | a0 |

Reaction conditions: styrene (10 mmol), TBHP (30 mmol), acetonitrile (10 mL); the

reactions were run for 6 h under reflux.

a The reaction was run for 10 h under reflux.

TABLE II. The influence of kind of oxidant on the oxidation of styrene

|  |  |  |  |
| --- | --- | --- | --- |
| **Entry** | **Catalyst** | **Oxidant** | **Conversion, %** |
| 1 | **1** | TBHP | 89 |
| 2 | **1** | H2O2 | 0 |

Reaction condition: styrene (10 mmol), catalyst (0.03 mmol), CH3CN (10 mL), oxidant

(30 mmol), reaction time (6 h) and reflux

TABLE III. Oxidation of styrene using TBHP catalyzed by **1** and CuL´-Y

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Entry** | **catalyst** | **Conversion, %** | **Selectivity, %** | | | | **Time, h** |
| 1 | **1** | 100 | a63 | b28 | | c9 | 6 |
| 2 | CuL´-Y | 100 | a56 | | b44 | | 4 |

Reaction conditions: catalyst (1:0.040 mmol, CuL´-Y: 0.04 g), styrene (10 mmol), TBHP (35 mmol), acetonitrile (10 mL) and reflux http://d.adroll.com/cm/r/outhttp://d.adroll.com/cm/x/outhttp://d.adroll.com/cm/l/out

a styrene epoxide

b benzoic acid

c benzaldehyde

TABLE IV. The influence of kind of oxidant on the oxidation of styrene

|  |  |  |  |
| --- | --- | --- | --- |
| **Entry** | **Catalyst** | **Oxidant** | **Conversion, %** |
| 1 | **3** | TBHP | 98 |
| 2 | **3** | H2O2 | 0 |

Reaction condition: styrene (10 mmol), catalyst (0.03 mmol), CH3CN (10 mL), oxidant

(35 mmol), reaction time (10 h) and reflux

TABLE V. Oxidation of styrene using TBHP catalyzed by **3** and **5**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Entry** | **Catalyst** | **Conversion, %** | **Selectivity, %** | |
| 1 | **3** | 100 | a47 | b53 |
| 2 | **5** | 40 | a46 | b54 |

Reaction conditions: catalyst (0.045 mmol), styrene (10 mmol), TBHP (35 mmol), acetonitrile

(10 mL), reaction time (10 h) and reflux

a styrene epoxide

b benzoic acid