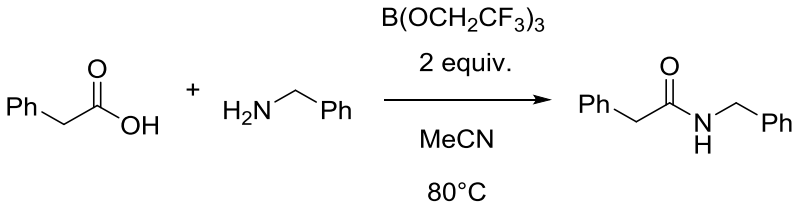
**Direct Amidation of carboxylic acids using a Borate Ester**

**Data Sheet**




*Org. Biomol. Chem.,* 2011, **9**, 1320

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**Experimental**

Tris(2,2,2-trifluoroethyl)borate (1.09g, 4mmol, 2 equivalents) was added to a solution/suspension of 2-phenylacetic acid (0.27g, 2mmol, 1 equivalent) and benzylamine (0.21g, 2mmol, 1 equivalent) in acetonitrile (4mL). The mixture was then heated at 80°C for 15 hours. The solvent was then removed under reduced pressure. The residue was dissolved in dichloromethane (30mL), washed with $NaHCO_3$ (1M) (20mL) and HCl (1M) (20mL) before drying over $MgSO_4$ (2g). The mixture was then filtered and concentrated under reduced pressure to give the clean product, N-benzyl-2-phenylacetamide (0.41g, 1.8mmol, 91% yield)

Adapted from *Org. Biomol. Chem.,* 2011, **9**, 1320. Some adaptations have been made: volumes and masses for some work-up chemicals have been estimated to allow metrics calculations. This has been done using best approximations based on the scale of the reaction where data was not provided.

**Risk Assessment** *(taken from MSDS)*

| Chemical | H-code | Description |
|---|---|---|
| tris(2,2,2-trifluoroethyl)borate | H226 | Flammable liquid and vapour |
| 2-phenylacetic acid | H315<br>H319<br>H335 | Skin irritation (Category 2)<br>Eye irritation (Category 2)<br>Specific target organ toxicity - single exposure (Category 3) |
| benzylamine | H302<br>H312<br>H314 | Harmful if swallowed<br>Harmful in contact with skin<br>Causes severe skin burns and eye damage |
| magnesium sulfate | none | - |
| acetonitrile | H225<br>H302<br>H332<br>H312<br>H319 | Flammable liquid (Category 2)<br>Acute toxicity, Oral (Category 4)<br>Acute toxicity, Inhalation (Category 4)<br>Acute toxicity, Dermal (Category 4)<br>Eye irritation (Category 2) |
| dichloromethane | H315<br>H319<br>H335<br>H336<br>H351<br>H373 | Causes skin irritation<br>Causes serious eye irritation<br>May cause respiratory irritation<br>May cause drowsiness or dizziness<br>Suspected of causing cancer<br>May cause damage to organs (Liver, Blood, Central nervous system) through prolonged or repeated exposure. |
| 1M sodium bicarbonate solution | none | - |
| 1M hydrochloric acid | H290 | May be corrosive to metals |

**Density of liquids** (g/mL at 25°C)

| | |
|---|---|
| acetonitrile | 0.786 |
| dichloromethane | 1.33 |
| Sodium bicarbonate (1M) | 1.10 |
| Hydrochloric acid (1M) | 1.017 |

**Boiling Points**

| | |
|---|---|
| acetonitrile | 82°C |
| dichloromethane | 40°C |

**Molecular weights of starting materials/product**

| | |
|---|---|
| 2-phenylacetic acid | 136.15 |
| benzylamine | 107.16 |
| N-benzyl-2-phenylacetamide | 225.29 |

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