Wood Protection Properties of Quaternary Ammonium Arylspiroborate Esters Derived from Naphthalene 2,3-diol, 2,2’-Biphenol and 3-Hydroxy-2-naphthoic acid


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- ACCESSORY PUBLICATION -

Geometry optimisations used for logP oct calculations.
Following methods used previously, the AM1 semi-empirical method, as implemented within the HyperChem Pro v7 package, was used to optimize all molecular geometries. This method was tested for its ability to reproduce the X-ray structure of NBu₄[B(bip)₂] (5). This method satisfactorily reproduced the experimentally observed tetrahedral spiroborate structure, as shown below (X-ray structure shown in green, AM1 in red). Table S1 gives selected geometrical parameters.

![Diagram showing the AM1 and X-ray structures of NBu₄[B(bip)₂] (5).]

**Table S1** Comparison of geometrical details for 5

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<thead>
<tr>
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<th>X-ray</th>
<th>AM1</th>
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<tbody>
<tr>
<td>B-O</td>
<td>1.465 – 1.475</td>
<td>1.444 – 1.478</td>
</tr>
<tr>
<td>C-O</td>
<td>1.366 – 1.373</td>
<td>1.361 – 1.370</td>
</tr>
<tr>
<td>B-N</td>
<td>5.03</td>
<td>4.78</td>
</tr>
<tr>
<td>Biphenyl dihedral</td>
<td>40.47, 47.5</td>
<td>36.7, 38.8</td>
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