New Sterically Hindered Tin(IV) Siloxane Precursors to Tinsilicate Materials:

Synthesis, Spectral, Structural and Photocatalytic Studies†‡

Mohan Gopalakrishnan\textsuperscript{a} and Nallasamy Palanisami\textsuperscript{a,*}

\textsuperscript{a}Materials Chemistry Division, School of Advanced Sciences, VIT University, Vellore 632 014, Tamil Nadu, India.

Corresponding author: E-mail: palanisami.n@gmail.com; Tel: +91 98426 39776; Fax no: +91416224 3092
Table S1. $^{119}$Sn and $^{29}$Si NMR chemical shift values for tin(IV) siloxanes 1–8.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>$\delta^{(119}\text{Sn})$ ppm</th>
<th>$\delta^{(29}\text{Si})$ ppm</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-149.60</td>
<td>-93.60</td>
<td>[1, 2]</td>
</tr>
<tr>
<td>2</td>
<td>-149.54</td>
<td>-93.37</td>
<td>[3, 1]</td>
</tr>
<tr>
<td>3</td>
<td>-148.98</td>
<td>-92.09</td>
<td>[4, 5]</td>
</tr>
<tr>
<td>4</td>
<td>-150.23</td>
<td>-91.62</td>
<td>[5, 6]</td>
</tr>
<tr>
<td>5</td>
<td>-151.31</td>
<td>-91.33</td>
<td>[7, 4]</td>
</tr>
<tr>
<td>6</td>
<td>-151.67</td>
<td>-91.32</td>
<td>[7, 2]</td>
</tr>
<tr>
<td>7</td>
<td>-151.34</td>
<td>-20.01</td>
<td>[8, 9]</td>
</tr>
<tr>
<td>8</td>
<td>-151.27</td>
<td>-20.08</td>
<td>[8, 9]</td>
</tr>
</tbody>
</table>

Figure S1. Geometry of tin and silicon in (t-Bu)$_2$Sn(OSi(Ot-Bu)$_3$)$_2$ (1).
Figure S2. Unit cell packing pattern in [(tBu)_2Sn(OSi(O^tBu)_3)_2] (1) hydrogen atoms are omitted for clarity.

Figure S3. Unit cell packing pattern in [(tBu)_2Sn(OSiPh_3)_2] (7) hydrogen atoms are omitted for clarity.
Figure S4. $^1$H NMR spectrum of [(tBu)$_2$Sn(OSi(OtBu)$_3$)$_2$] (1) in CDCl$_3$.

Figure S5. $^{13}$C NMR spectrum of [(tBu)$_2$Sn(OSi(OtBu)$_3$)$_2$] (1) in CDCl$_3$. 
Figure S6. $^{29}$Si NMR spectrum of [(t'Bu)$_2$Sn(OSi(Ot'Bu)$_3$)$_2$] 1 in CDCl$_3$.

Figure S7. $^{119}$Sn NMR spectrum of [(t'Bu)$_2$Sn(OSi(Ot'Bu)$_3$)$_2$] 1 in C$_6$D$_6$. 
Figure S8. $^{29}$Si NMR spectrum of $[\{t^6\text{Bu}\}_2\text{Sn(O}(O\text{Bu})_3\text{Cl}\}]$ (2) in C$_6$D$_6$.

Figure S9. $^{119}$Sn NMR spectrum of $[\{t^6\text{Bu}\}_2\text{Sn(O}(O\text{Bu})_3\text{Cl}\}]$ (2) in C$_6$D$_6$. 
Figure S10. $^1$H NMR spectrum of $[(n$-Bu)$_2$Sn(OSi(O$_{\text{t}}$Bu)$_3$)$_2$] (3) in C$_6$D$_6$.

Figure S11. $^{13}$C NMR spectrum of $[(n$-Bu)$_2$Sn(OSi(O$_{\text{t}}$Bu)$_3$)$_2$] (3) in C$_6$D$_6$. 
Figure S12. $^{29}$Si NMR spectrum of [(n-Bu)$_2$Sn(OSi(OtBu)$_3$)$_2$] (3) in C$_6$D$_6$.

Figure S13. $^1$H NMR spectrum of [(n-Bu)$_2$Sn(OSi(OtBu)$_3$)Cl] (4) in CDCl$_3$. 
**Figure S14.** $^{13}$C NMR spectrum of [(n-Bu)$_2$Sn(OSi(O'Bu)$_3$)Cl] (4) in CDCl$_3$.

**Figure S15.** $^{29}$Si NMR spectrum of [(n-Bu)$_2$Sn(OSi(O'Bu)$_3$)Cl] (4) in C$_6$D$_6$. 
Figure S16. $^1$H NMR spectrum of $[(\text{Me})_2\text{Sn(OSi(O}^\text{t}\text{Bu})_3)_2]$ (5) in C$_6$D$_6$.

Figure S17. $^{13}$C NMR spectrum of $[(\text{Me})_2\text{Sn(OSi(O}^\text{t}\text{Bu})_3)_2]$ (5) in C$_6$D$_6$. 
Figure S18. $^{29}$Si NMR spectrum of [((Me)$_2$Sn(OSi(O$^t$Bu)$_3$)$_2$] (5) in C$_6$D$_6$.

Figure S19. $^{119}$Sn NMR spectrum of [((Me)$_2$Sn(OSi(O$^t$Bu)$_3$)$_2$] (5) in C$_6$D$_6$. 
Figure S20. $^1$H NMR spectrum of $[(\text{Me})_2\text{Sn(OSi(O}^\text{t} \text{Bu})_3]\text{Cl}]$ (6) in CDCl$_3$.

Figure S21. $^{13}$C NMR spectrum of $[(\text{Me})_2\text{Sn(OSi(O}^\text{t} \text{Bu})_3]\text{Cl}]$ (6) in CDCl$_3$. 
Figure S22. $^{29}$Si NMR spectrum of [(Me)$_2$Sn(OSi(O'Bu)$_3$)Cl] (6) in C$_6$D$_6$.

Figure S23. $^1$H NMR spectrum of [(tBu)$_2$Sn(OSiPh$_3$)$_2$] (7) in CDCl$_3$. 
Figure S24. $^{13}$C NMR spectrum of [(tBu)$_2$Sn(OSiPh$_3$)$_2$] (7) in CDCl$_3$.

Figure S25. $^{29}$Si NMR spectrum of [(tBu)$_2$Sn(OSiPh$_3$)$_2$] (7) in CDCl$_3$. 
Figure S26. $^{119}$Sn NMR spectrum of $[({}^t\text{Bu})_2\text{Sn(OSiPh}_3)_2]$ (7) in CDCl$_3$.

Figure S27. $^{29}$Si NMR spectrum of $[({}^t\text{Bu})_2\text{Sn(OSiPh}_3)_2\text{Cl}]$ (8) in C$_6$D$_6$. 
Figure S28. $^{119}$Sn NMR spectrum of [(t-Bu)$_2$Sn(OSiPh$_3$)Cl] (8) in C$_6$D$_6$. 
Figure S29. FT-IR spectrum of [(tBu)₂Sn(OSi(tBu)₃)₂] (1).
Figure S30. FT-IR spectrum of [(n-Bu)$_2$Sn(OSi(O'tBu)$_3$)$_2$] (3).

Figure S31. FT-IR spectrum of [(Me)$_2$Sn(OSi(O'Bu)$_3$)$_2$] (5).
Figure S32. FT-IR spectrum of [(‘Bu)_2Sn(OSiPh_3)_2] (7)

Figure S33. Powder XRD patterns of the tinsilicate material obtained from degradation of 1.
References


