# Supplementary Materials: Preparation and DFT Studies of κ²*C,N*-Hypercoordinated Oxazoline Organotins: Monomer Constructs for Stable Polystannanes

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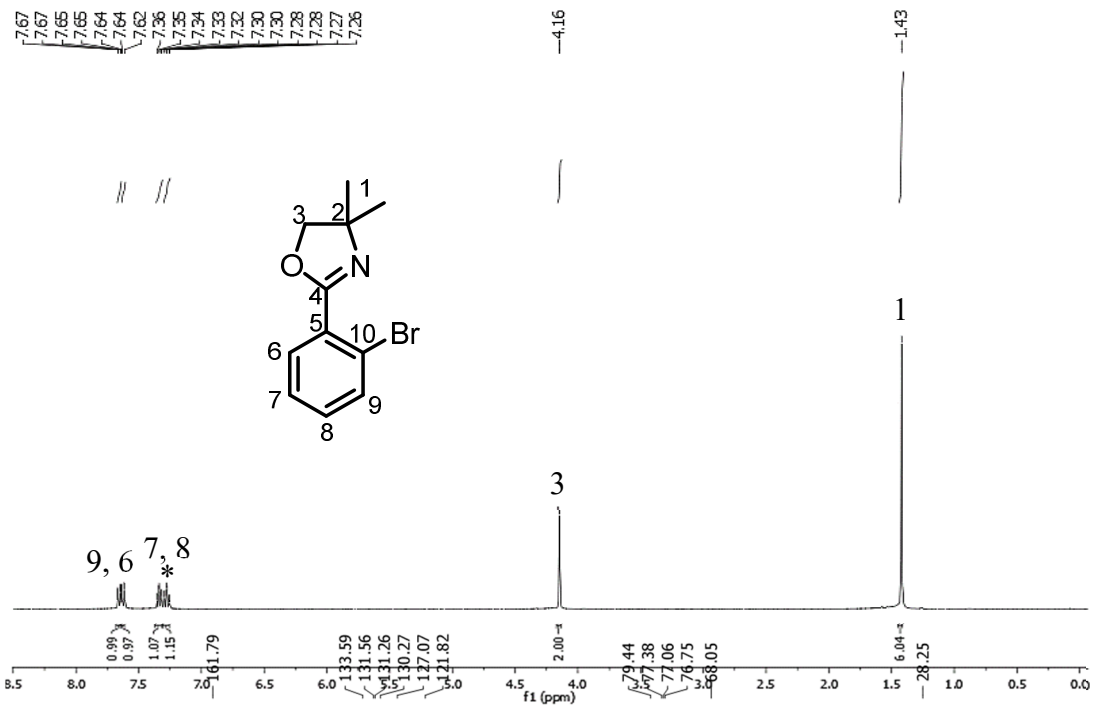


**Figure S1:** $^{1}$H NMR spectrum of **5** in $CDCl_3$*.

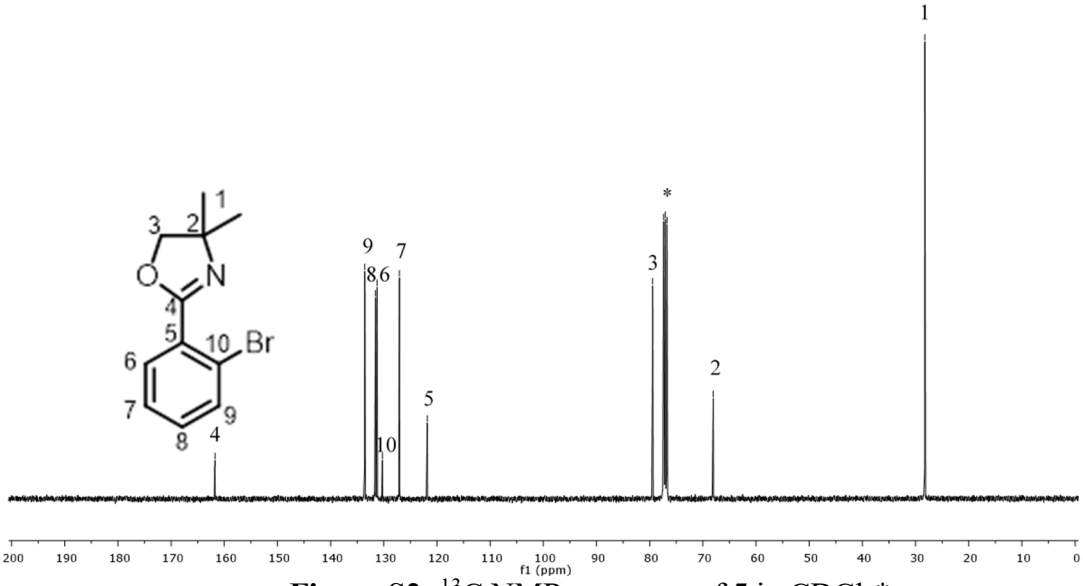


**Figure S2:** $^{13}$C NMR spectrum of **5** in $CDCl_3$*.

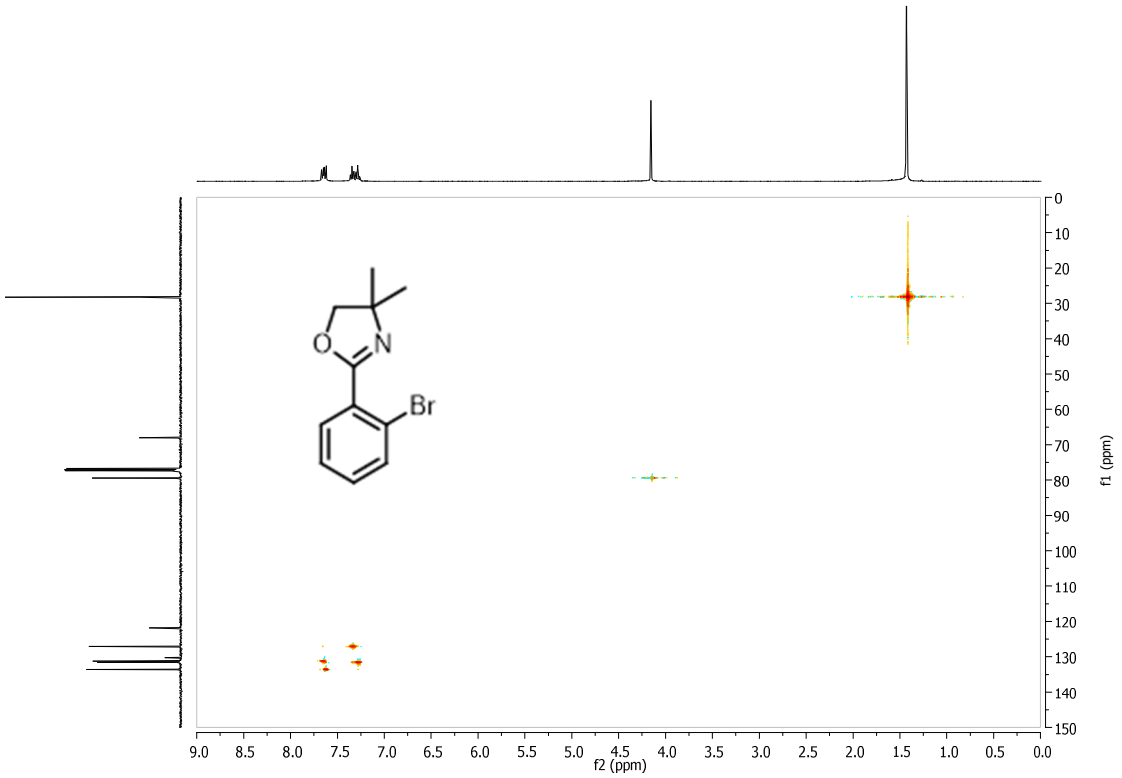


**Figure S3:** HSQC spectrum of **5** in $CDCl_3$.

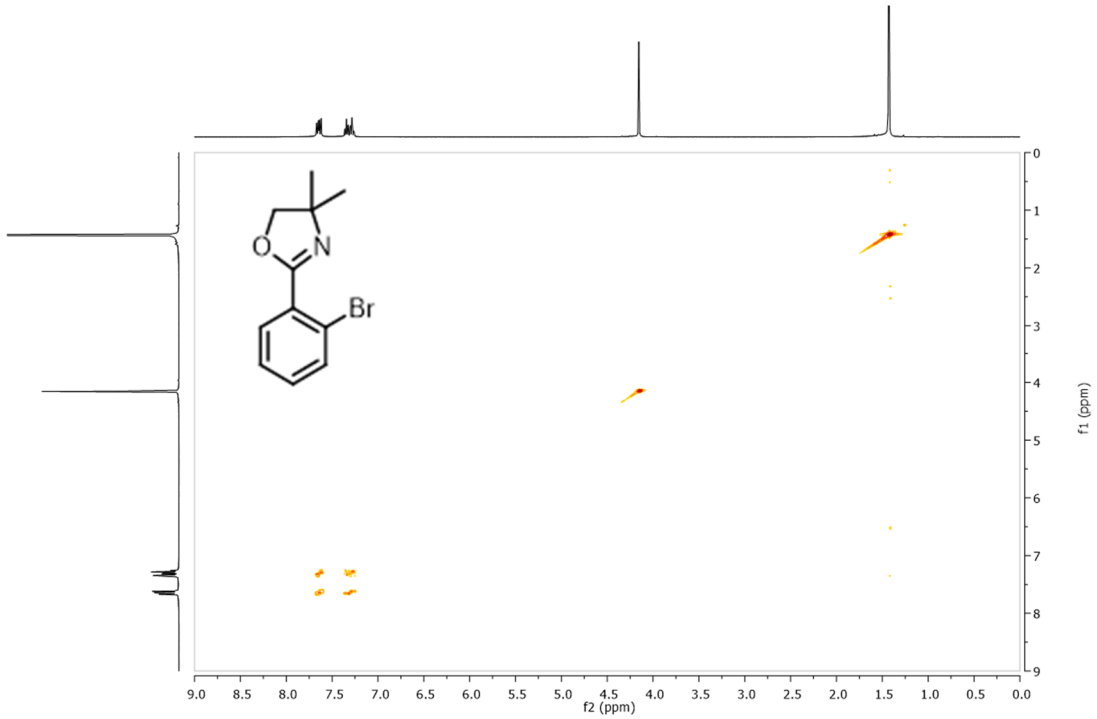


**Figure S4:** COSY spectrum of **5** in $CDCl_3$.

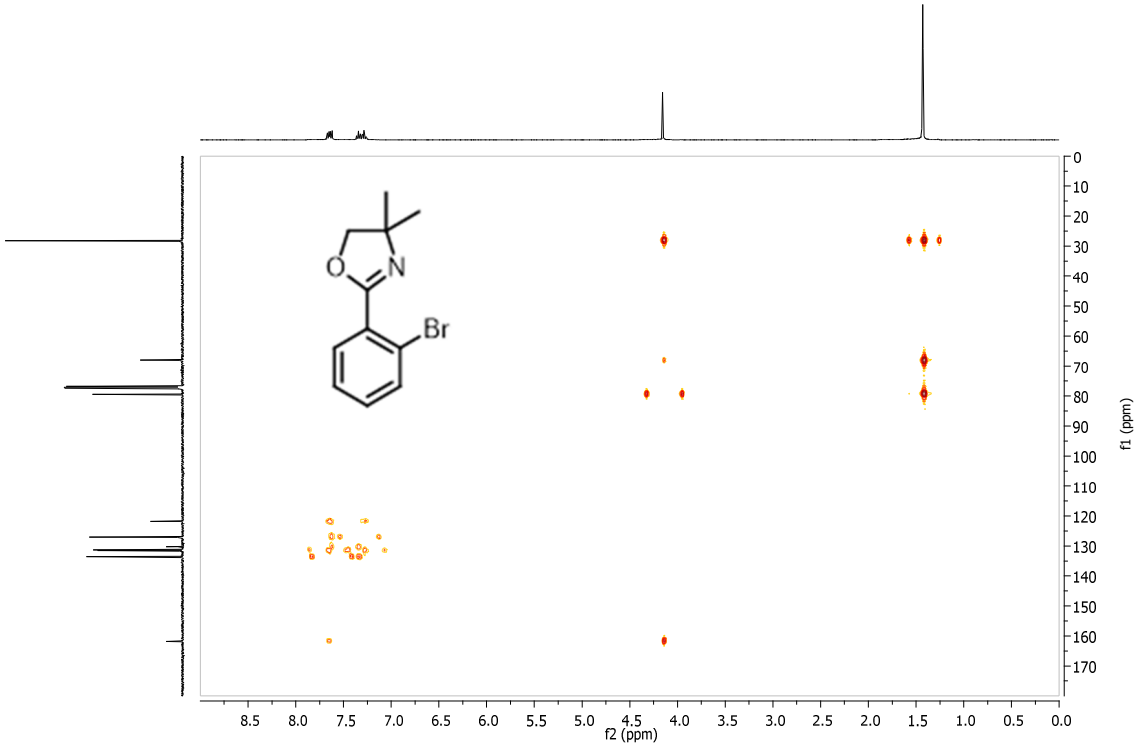


**Figure S5:** HMBC spectrum of **5** in $CDCl_3$.

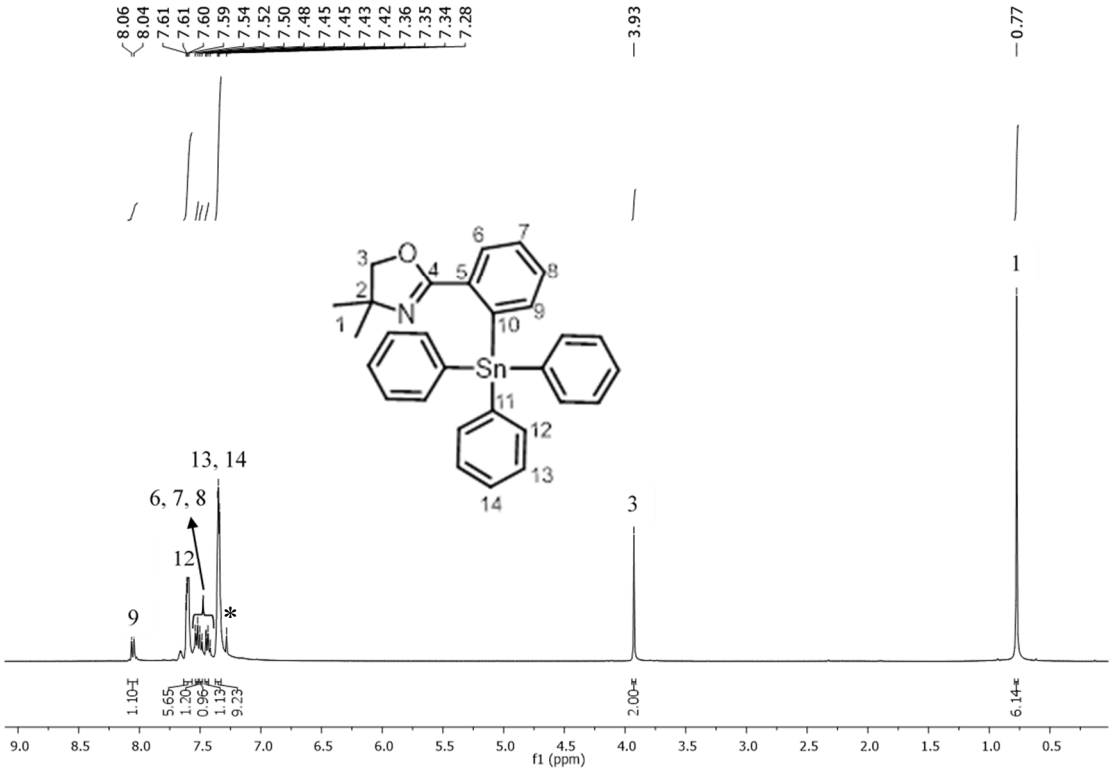


**Figure S6**: $^1$H NMR spectrum of **7** in $CDCl_3$*.

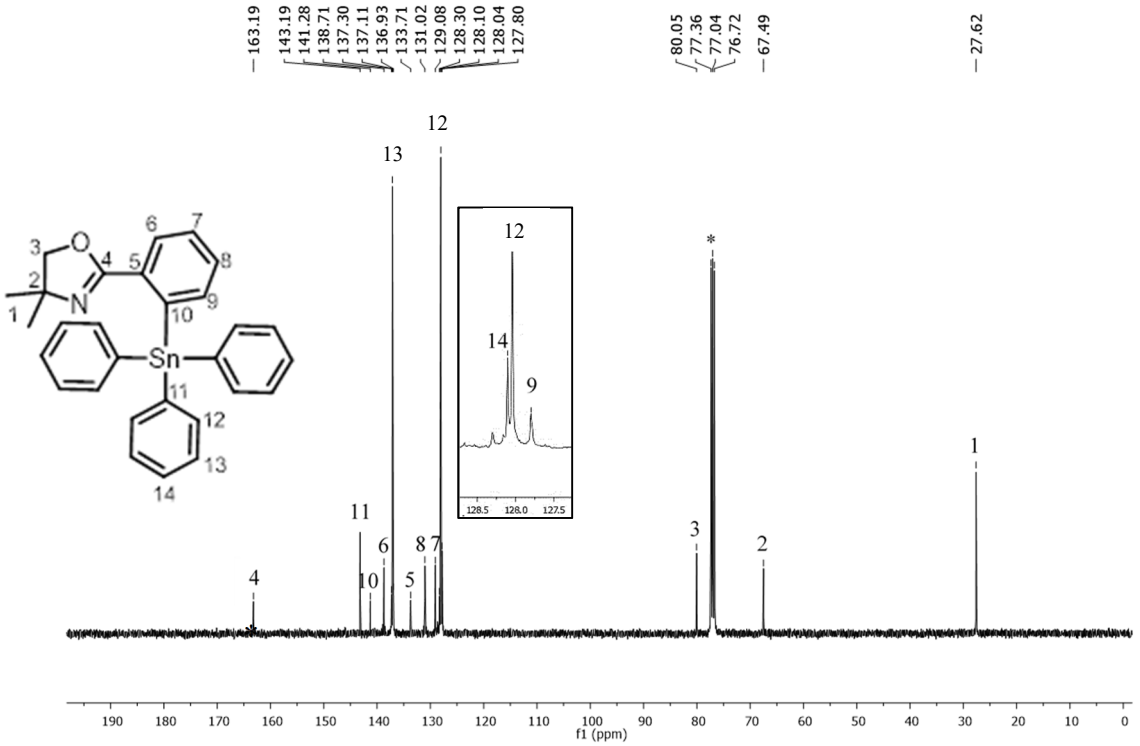


**Figure S7:** $^{13}$C NMR spectrum of **7** in $CDCl_3$*.

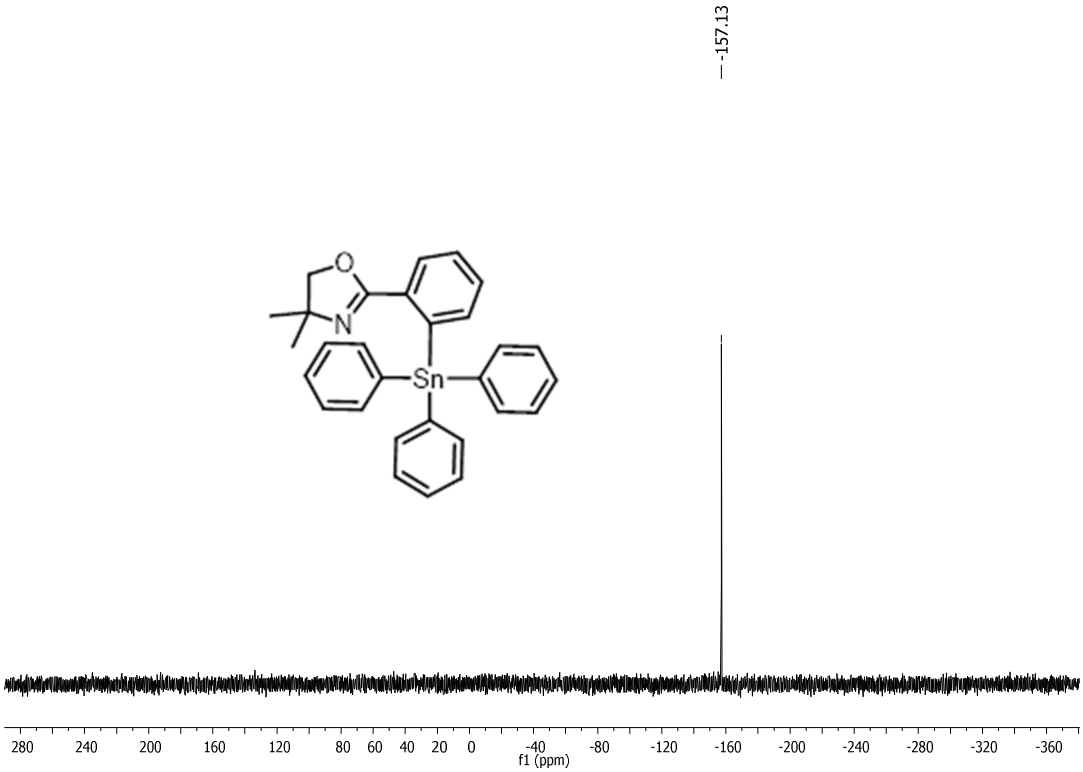


**Figure S8:** $^{119}$Sn NMR spectrum of **7** in $CDCl_3$.

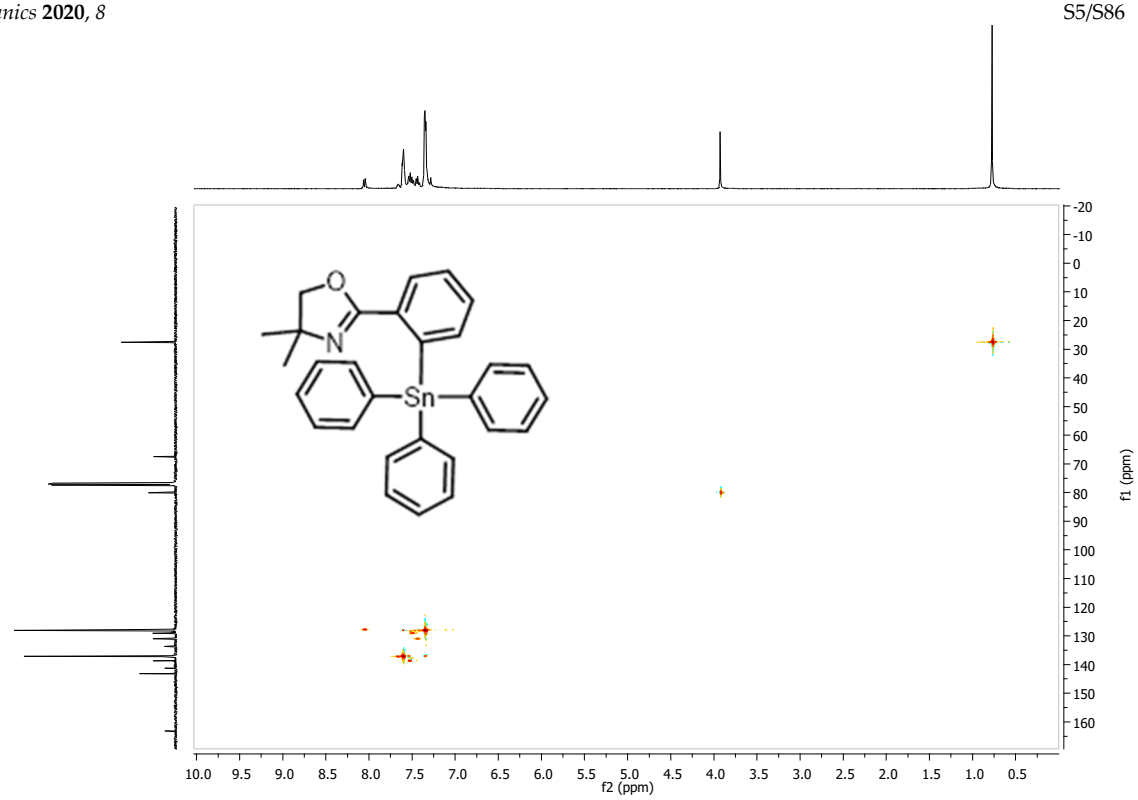


**Figure S9:** HSQC spectrum of **7** in $CDCl_3$.

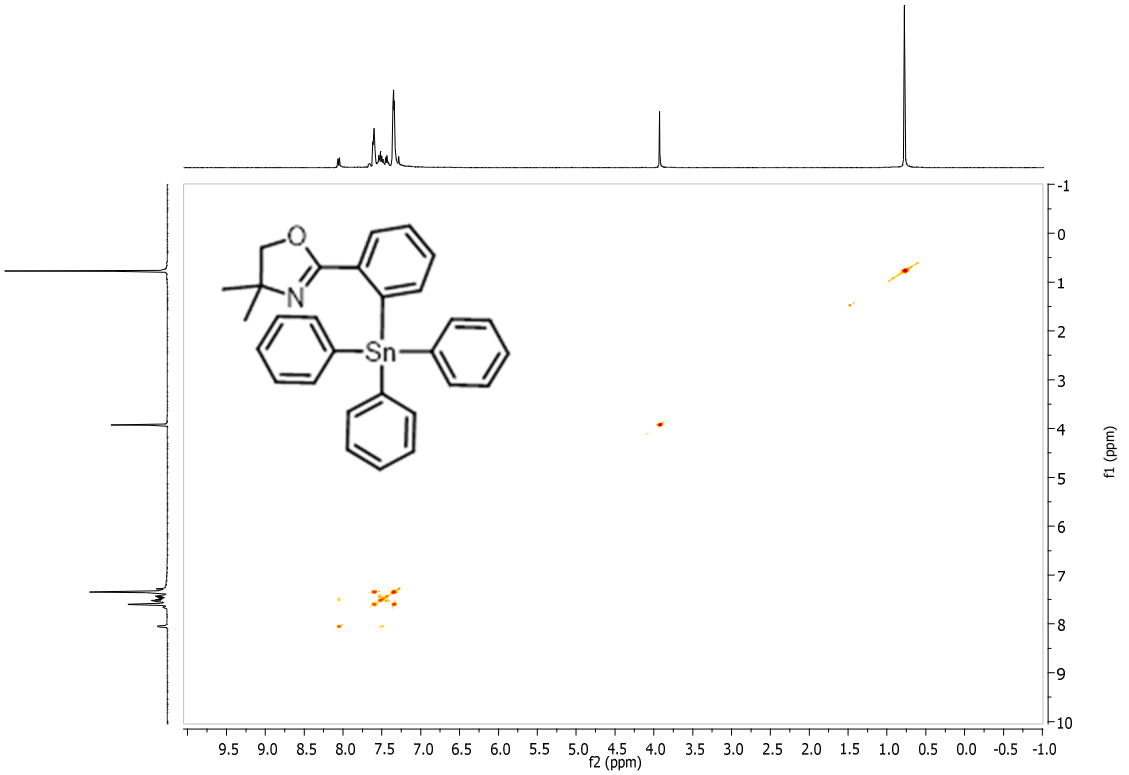


**Figure S10:** COSY spectrum of **7** in $CDCl_3$.

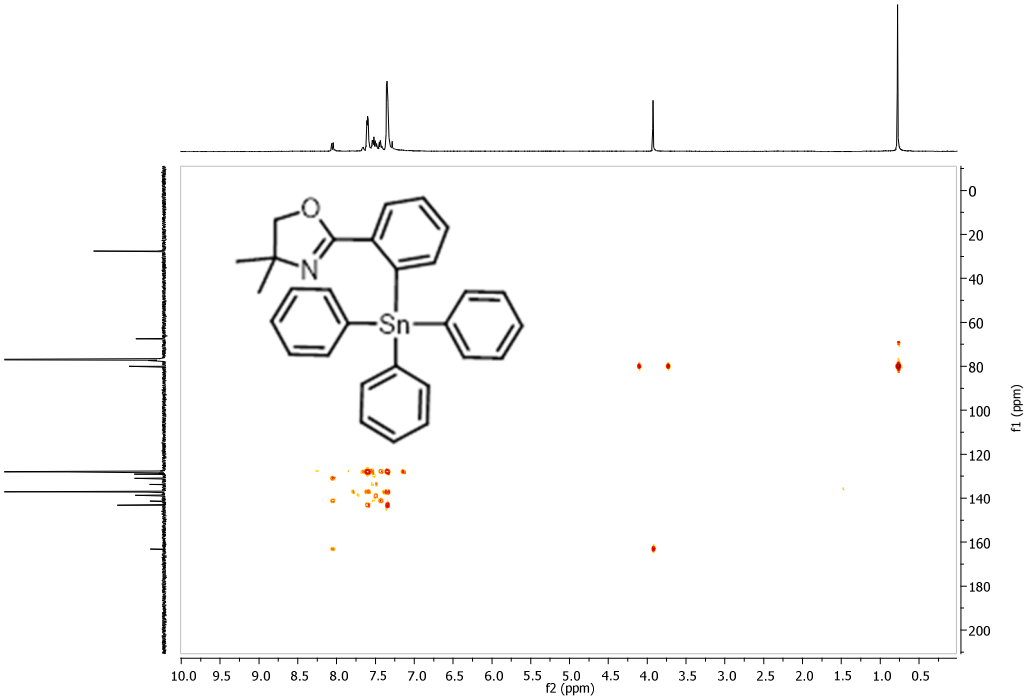


**Figure S11:** HMBC spectrum of **7** in $CDCl_3$.

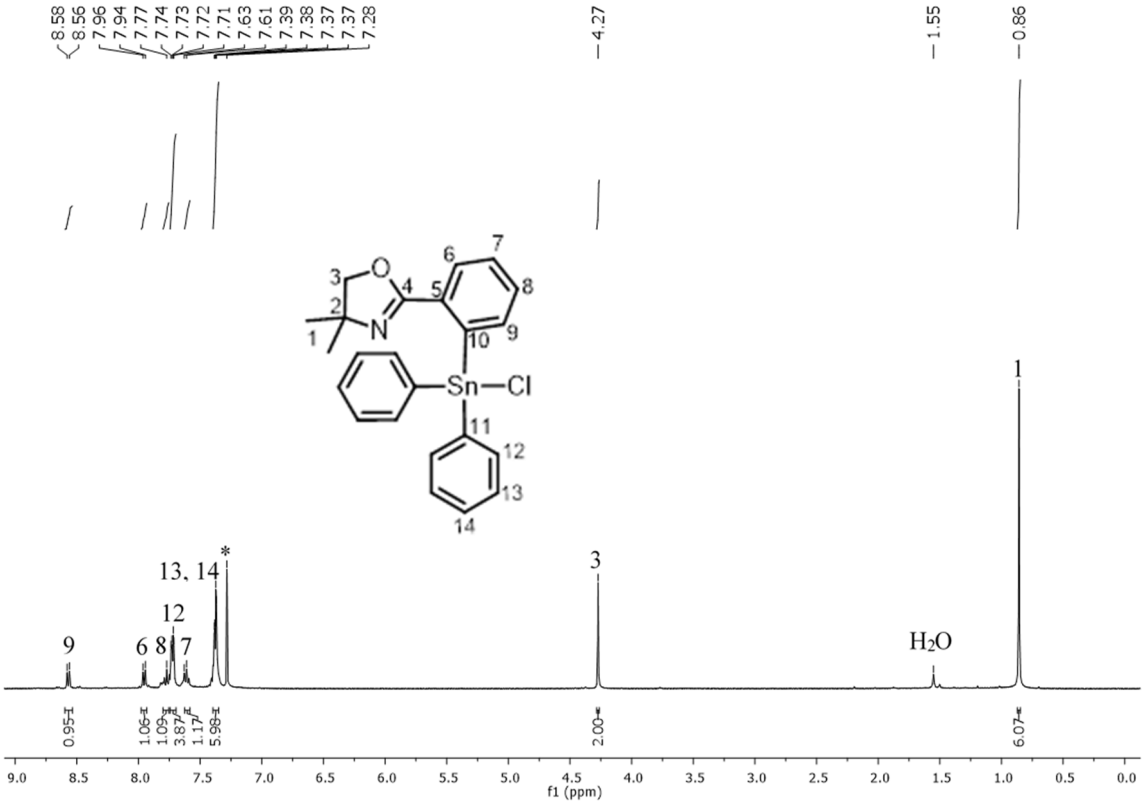


**Figure S12:** $^1$H NMR spectrum of **9** in $CDCl_3$*.

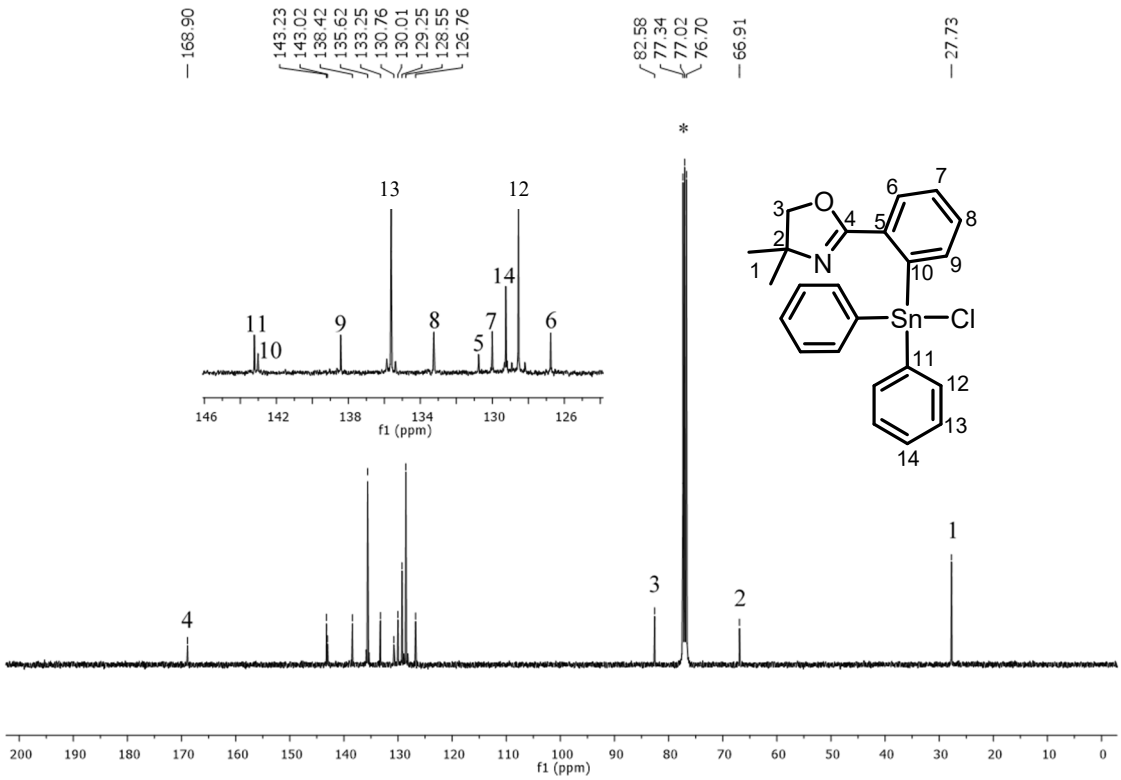


**Figure S13:** $^{13}$C NMR spectrum of **9** in $CDCl_3$*.

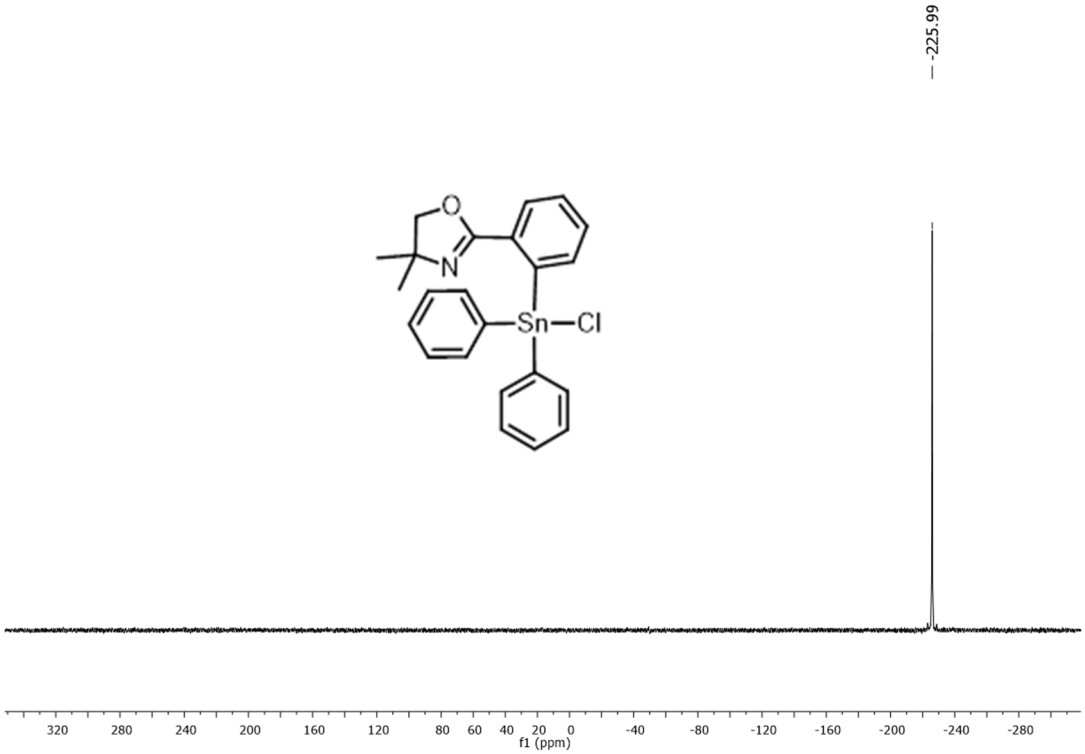


**Figure S14:** $^{119}$Sn NMR spectrum of **9** in $CDCl_3$.

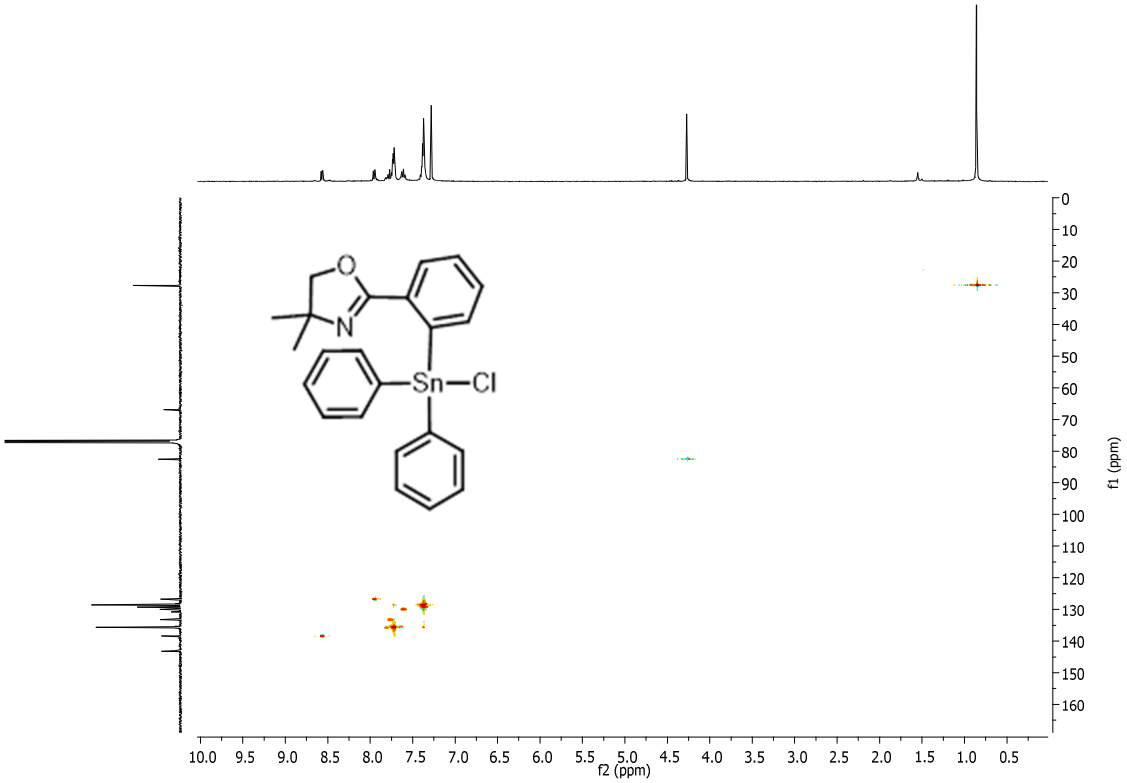


**Figure S15:** HSQC spectrum of **9** in $CDCl_3$.

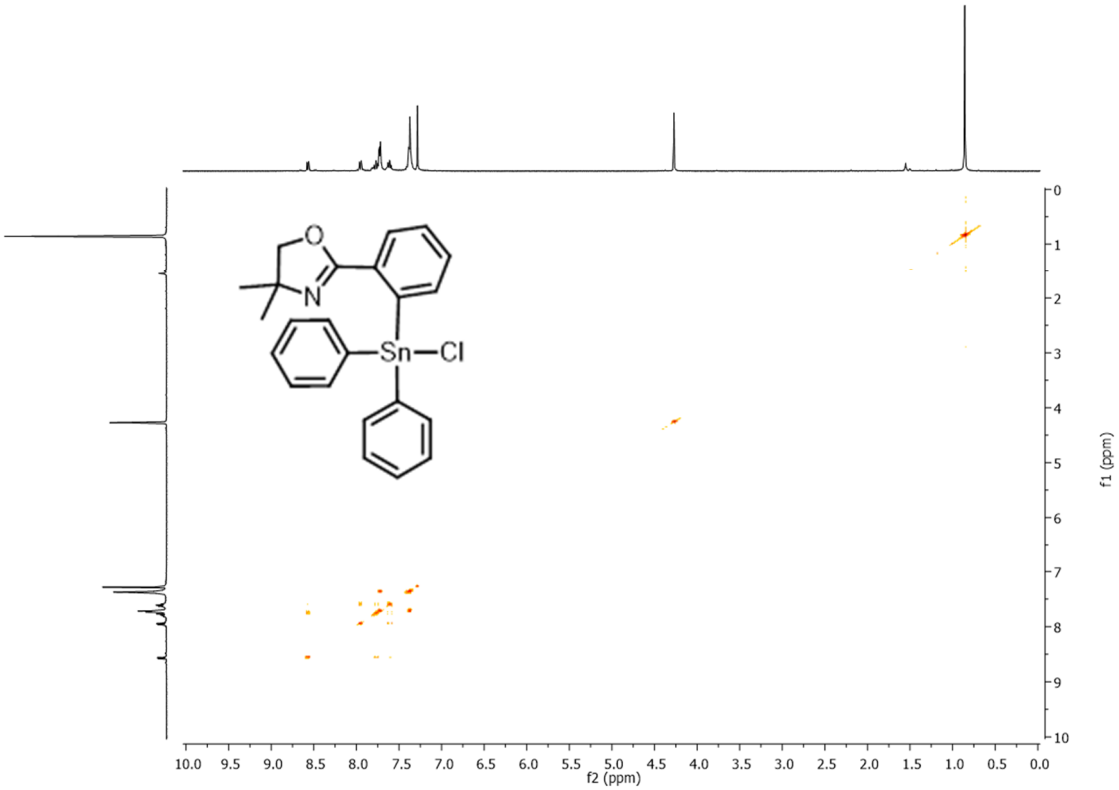


**Figure S16:** COSY spectrum of **9** in $CDCl_3$.

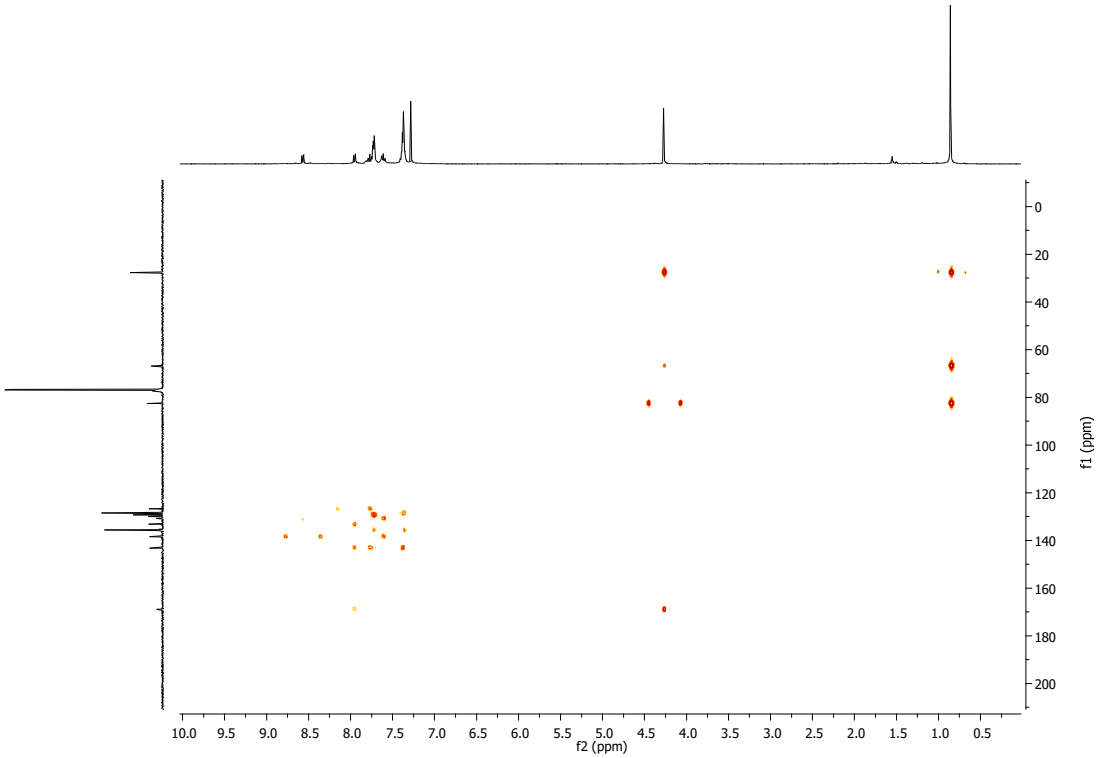


**Figure S17:** HMBC spectrum of **9** in $CDCl_3$.

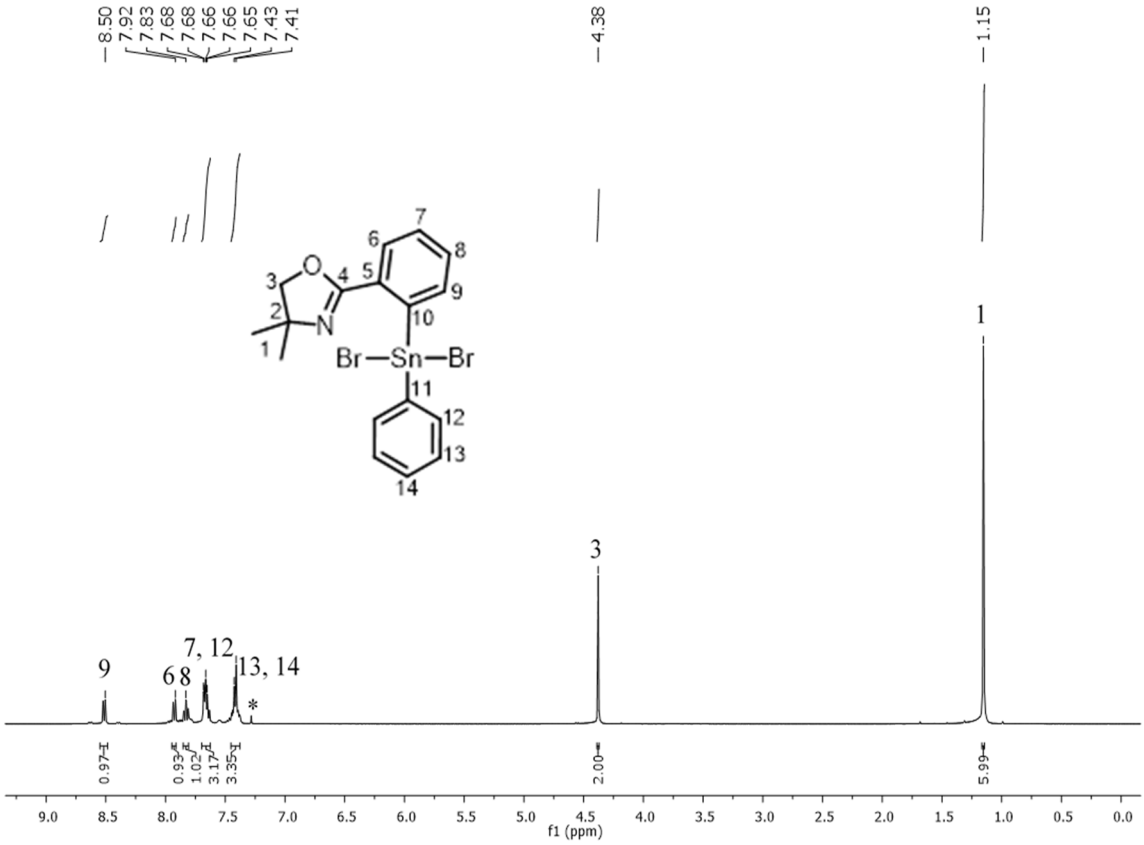


**Figure S18:** $^1$H NMR spectrum of **10** in $CDCl_3$.

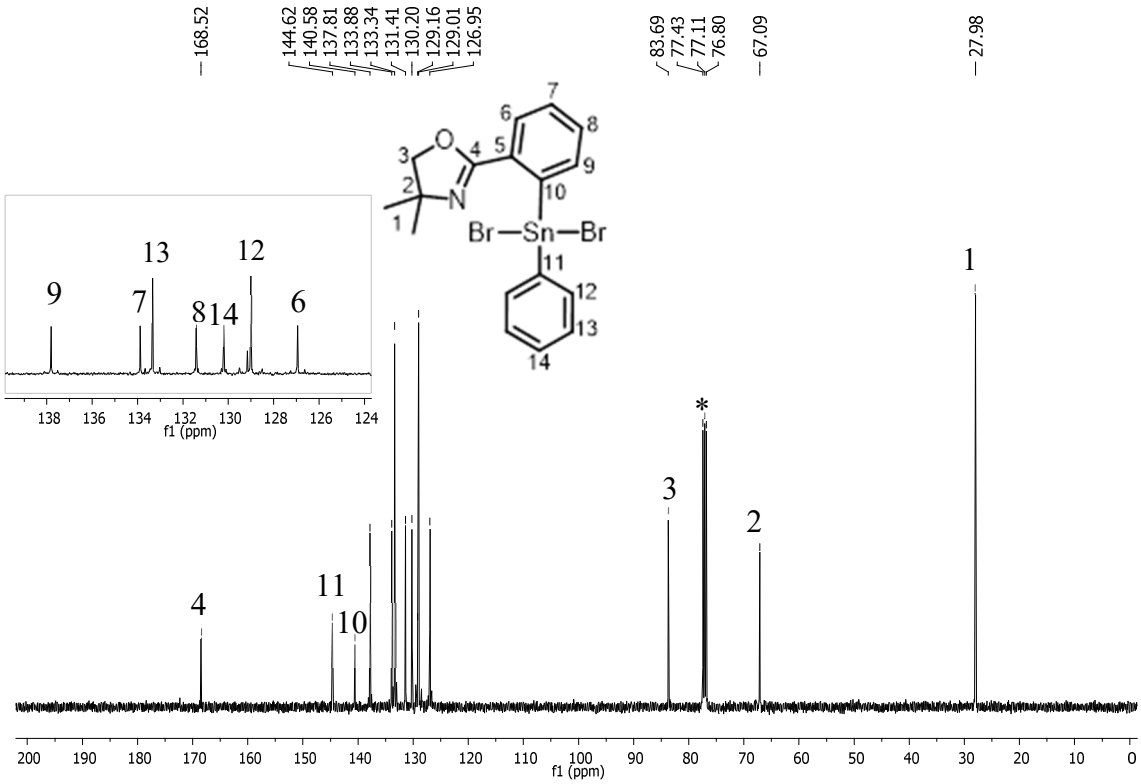


**Figure S19:** $^{13}$C NMR spectrum of **10** in $CDCl_3$*.

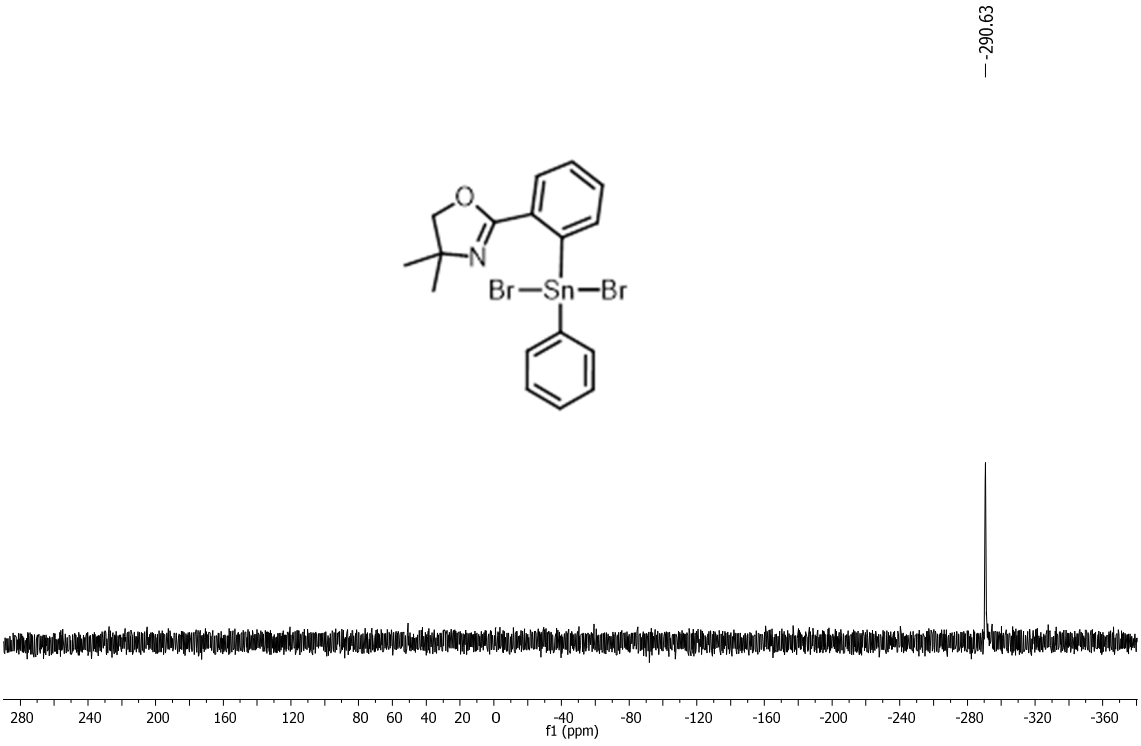


**Figure S20:** $^{119}$Sn NMR spectrum of **10** in $CDCl_3$.

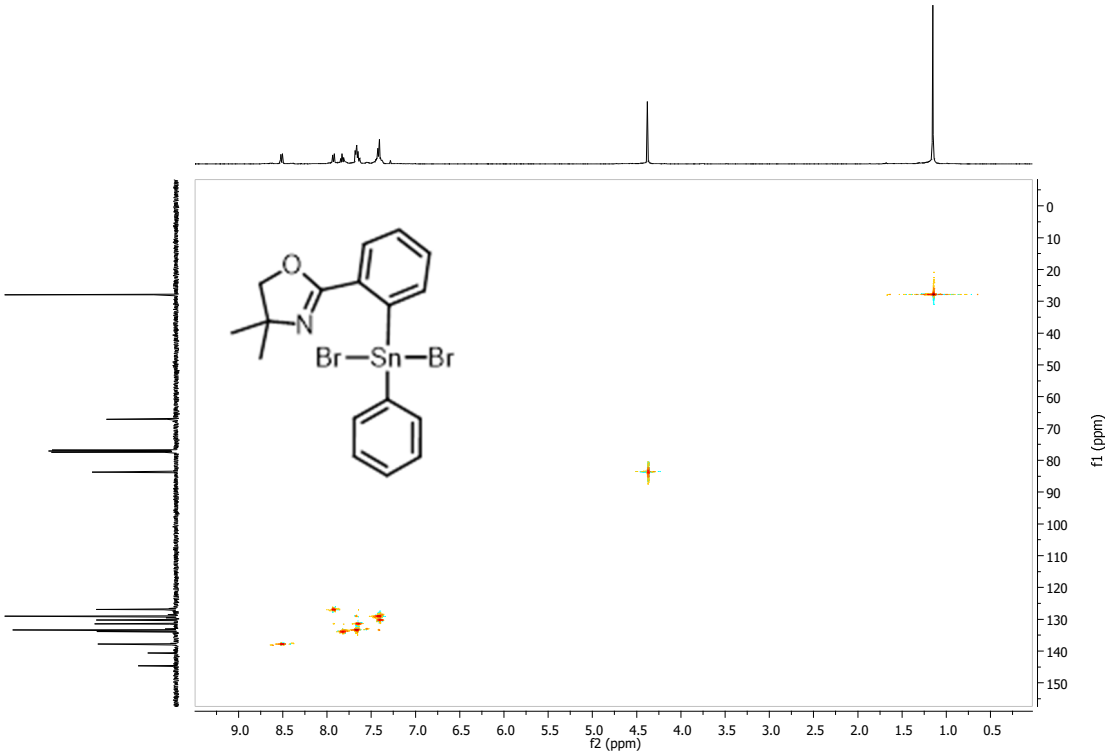


**Figure S21:** HSQC spectrum of **10** in $CDCl_3$.

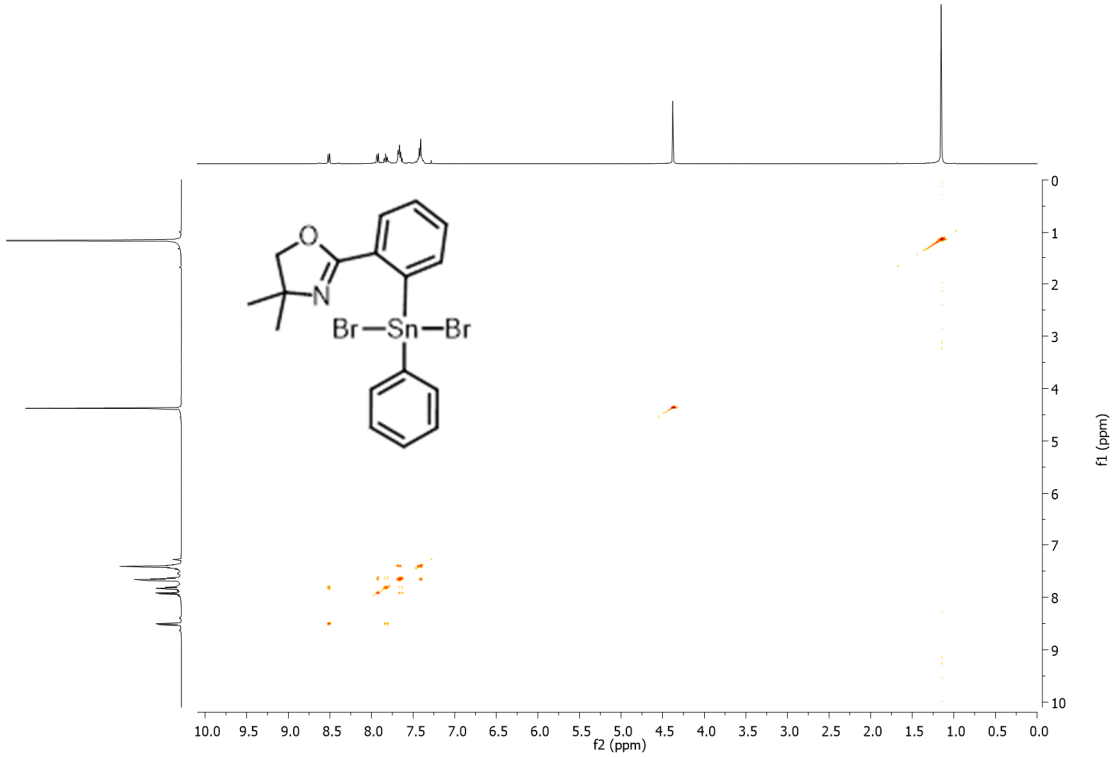


**Figure S22:** COSY spectrum of **10** in $CDCl_3$.

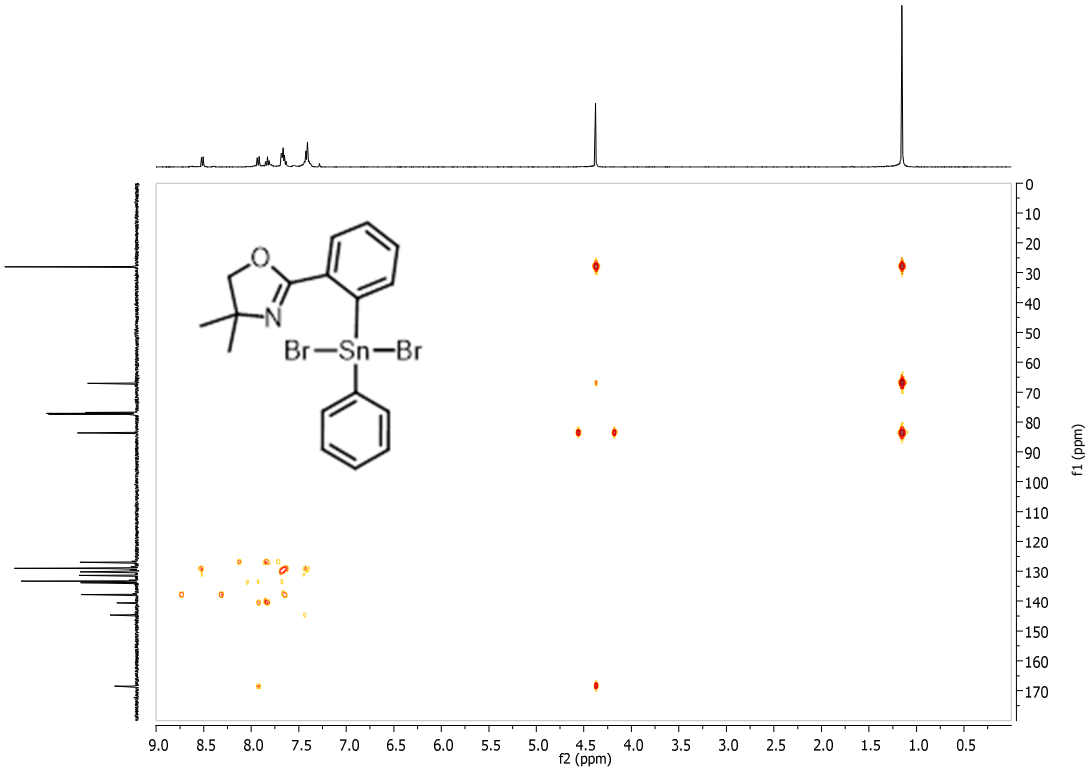


**Figure S23:** HMBC spectrum of **10** in $CDCl_3$.

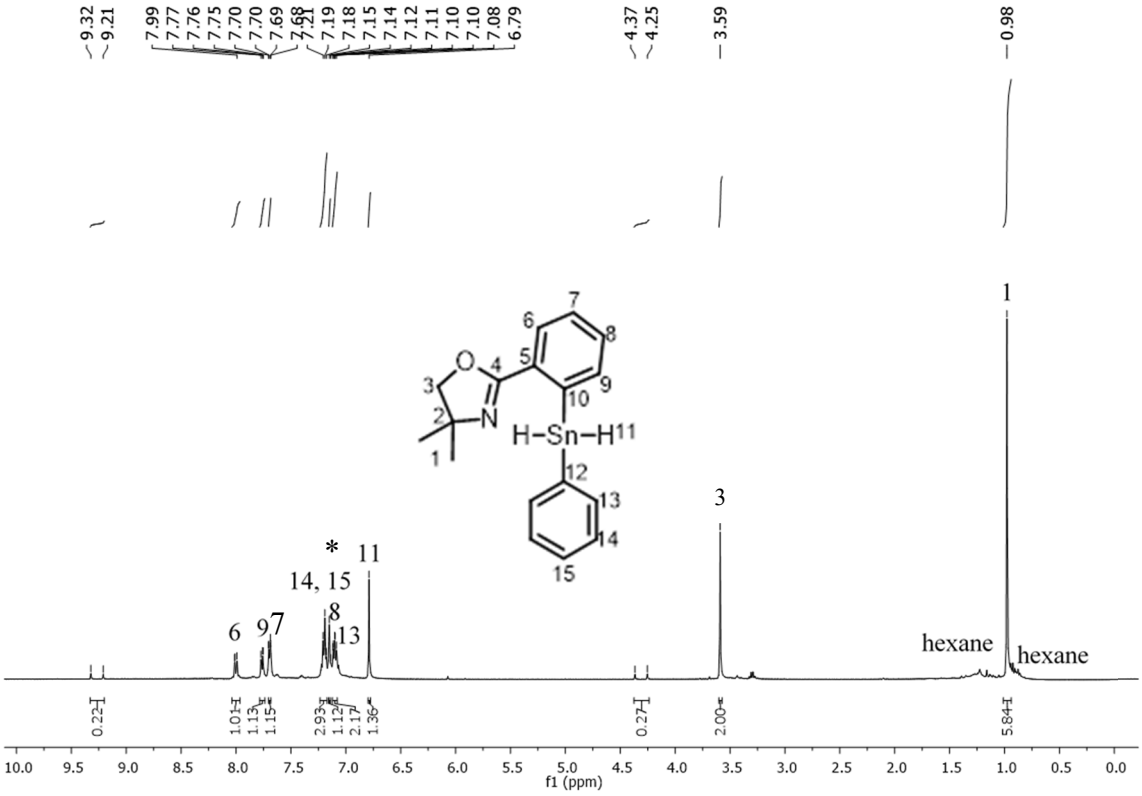


**Figure S24:** $^1$H NMR spectrum of **12** in $C_6D_6$*.

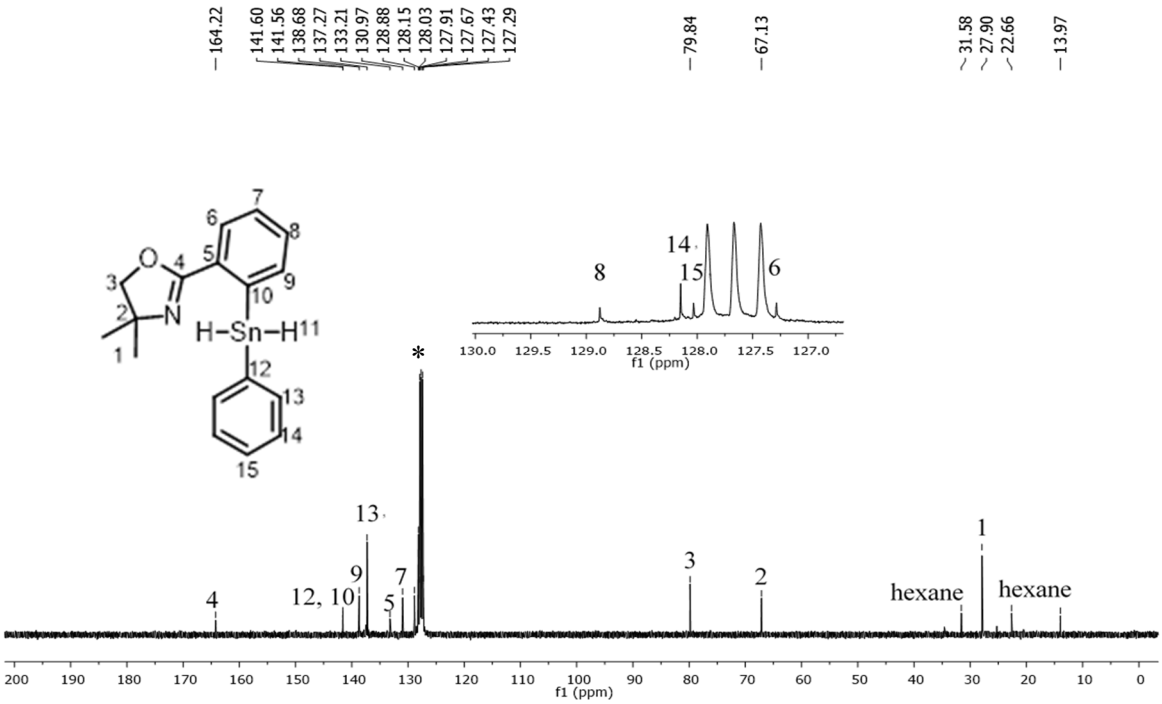


**Figure S25:** $^{13}$C NMR spectrum of **12** in $C_6D_6$*.

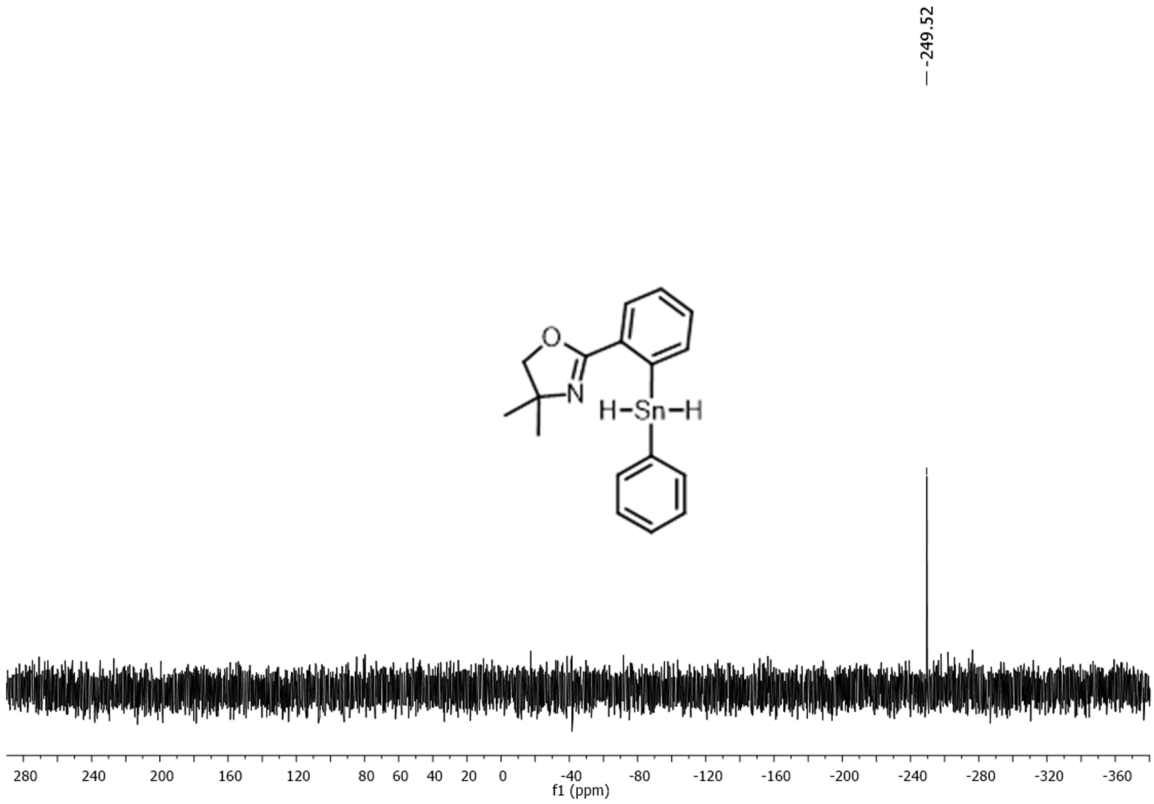


**Figure S26:** $^{119}$Sn NMR spectrum of **12** in $C_6D_6$.

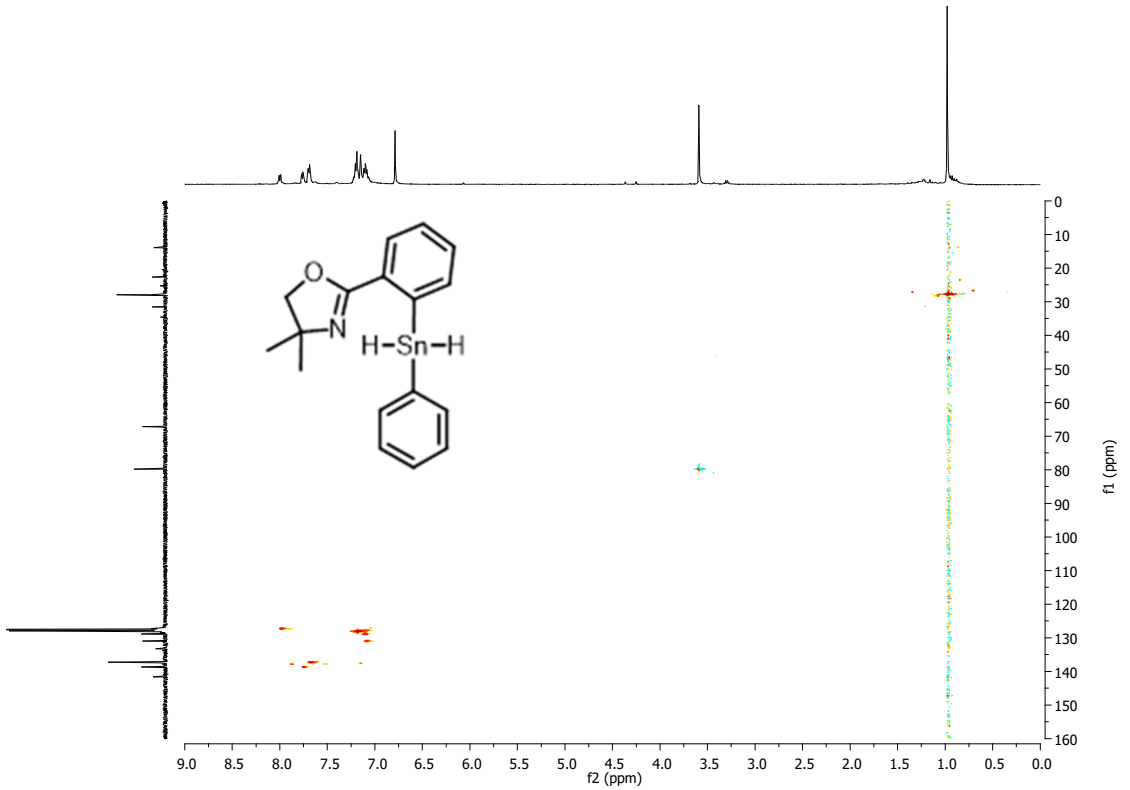


**Figure S27:** HSQC spectrum of **12** in $C_6D_6$.

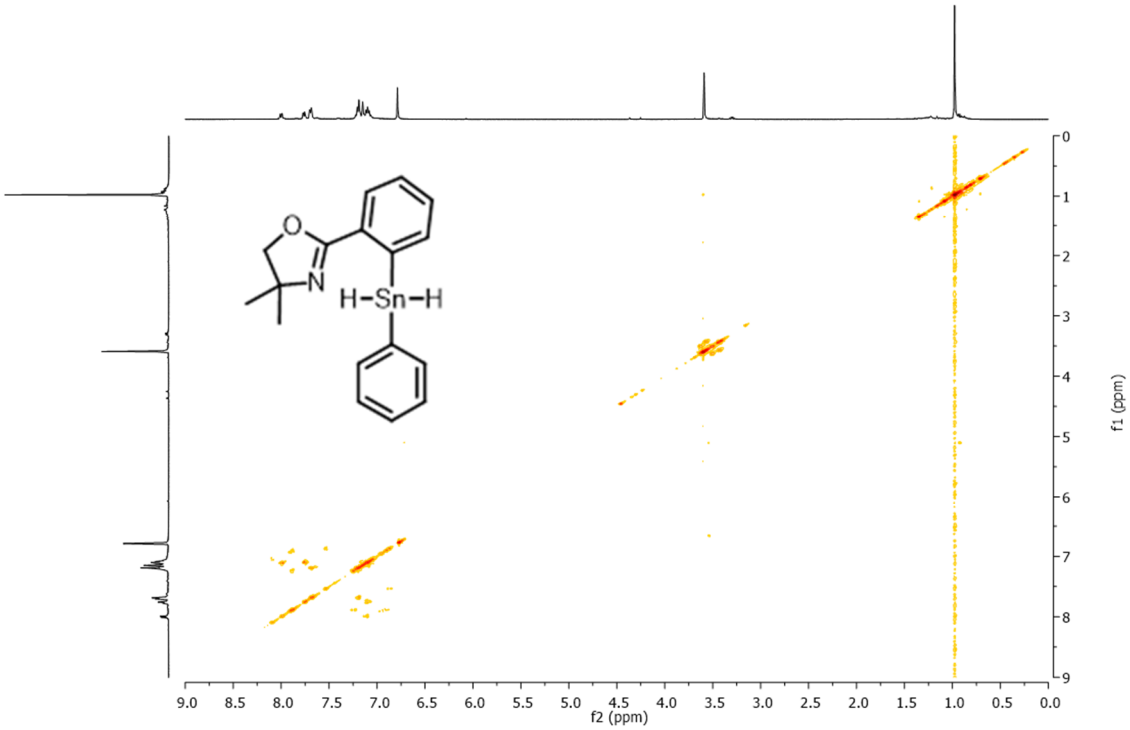


**Figure S28:** COSY spectrum of **12** in $C_6D_6$.

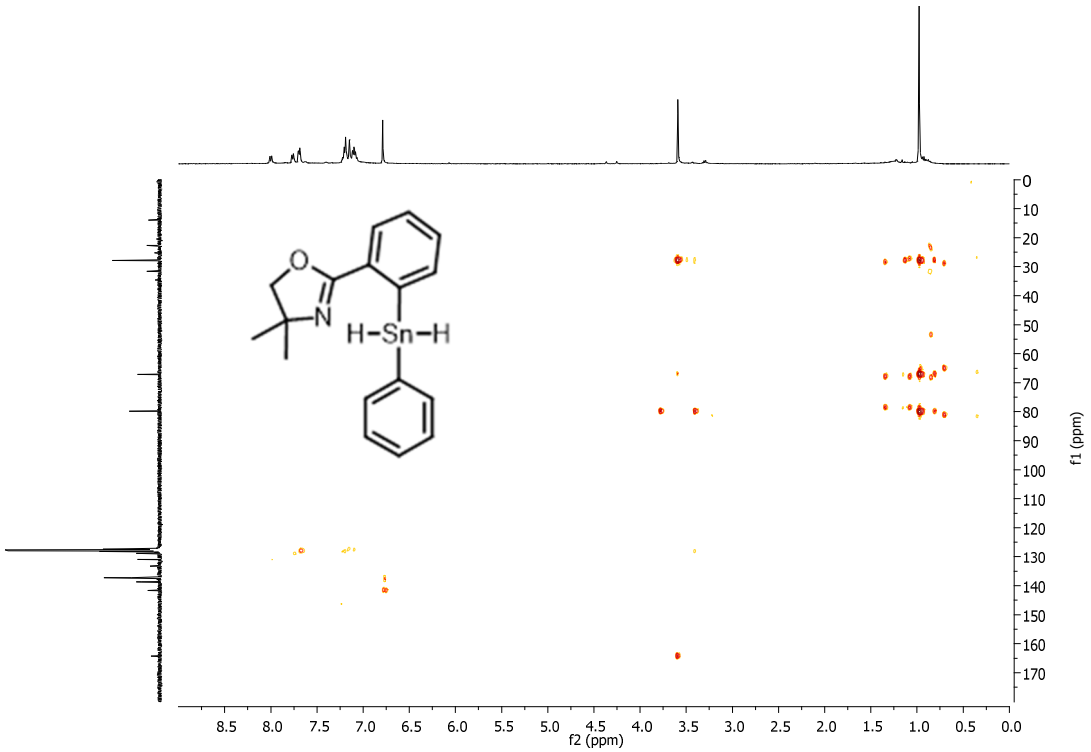


**Figure S29:** HMBC spectrum of **12** in $C_6D_6$.

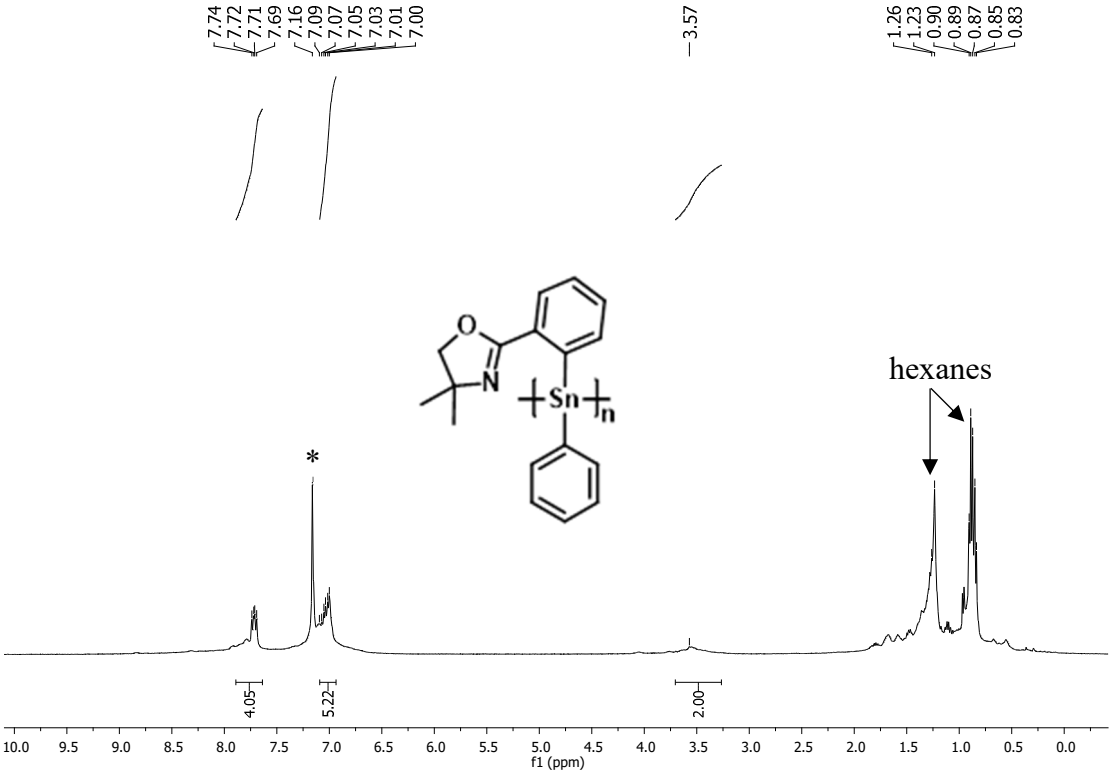


**Figure S30:** $^1$H NMR spectrum of **14** in $C_6D_6$*.

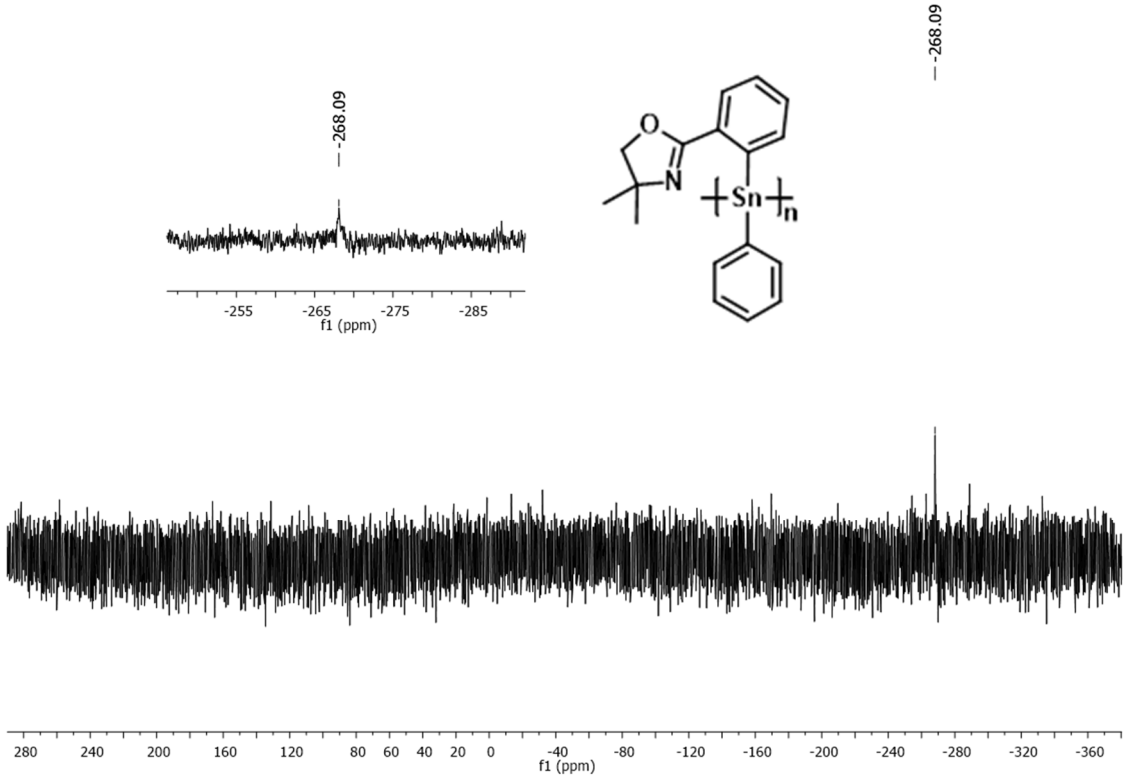


**Figure S31:** $^{119}$Sn NMR spectrum of **14** in $C_6D_6$.

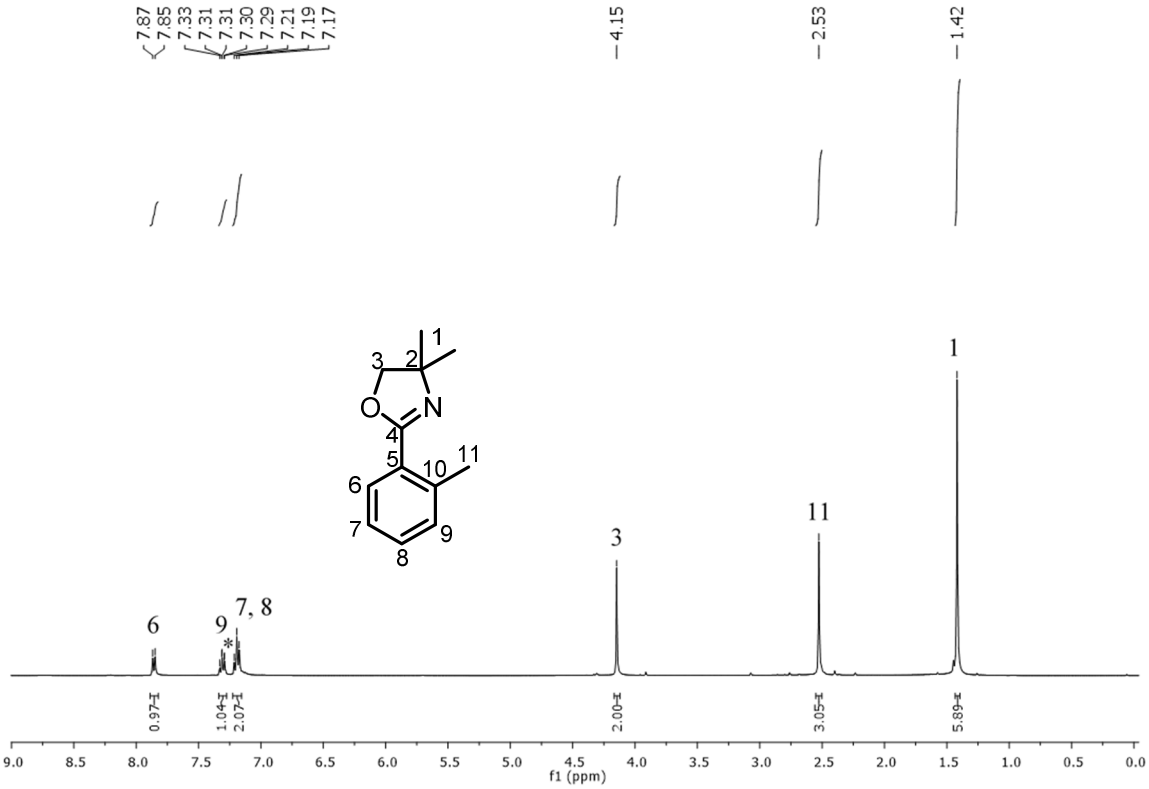


**Figure S32:** $^{1}$H NMR spectrum of **8** in $CDCl_3$*.

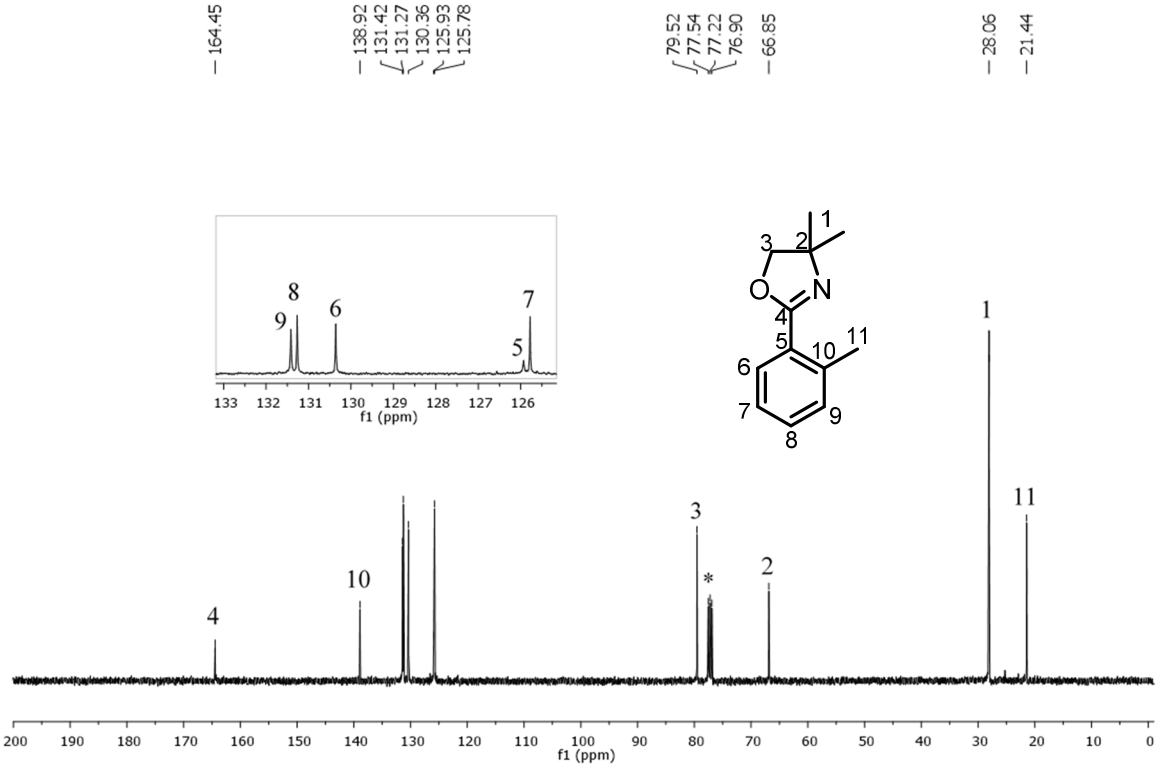


**Figure S33:** $^{13}$C NMR spectrum of **8** in $CDCl_3$*.

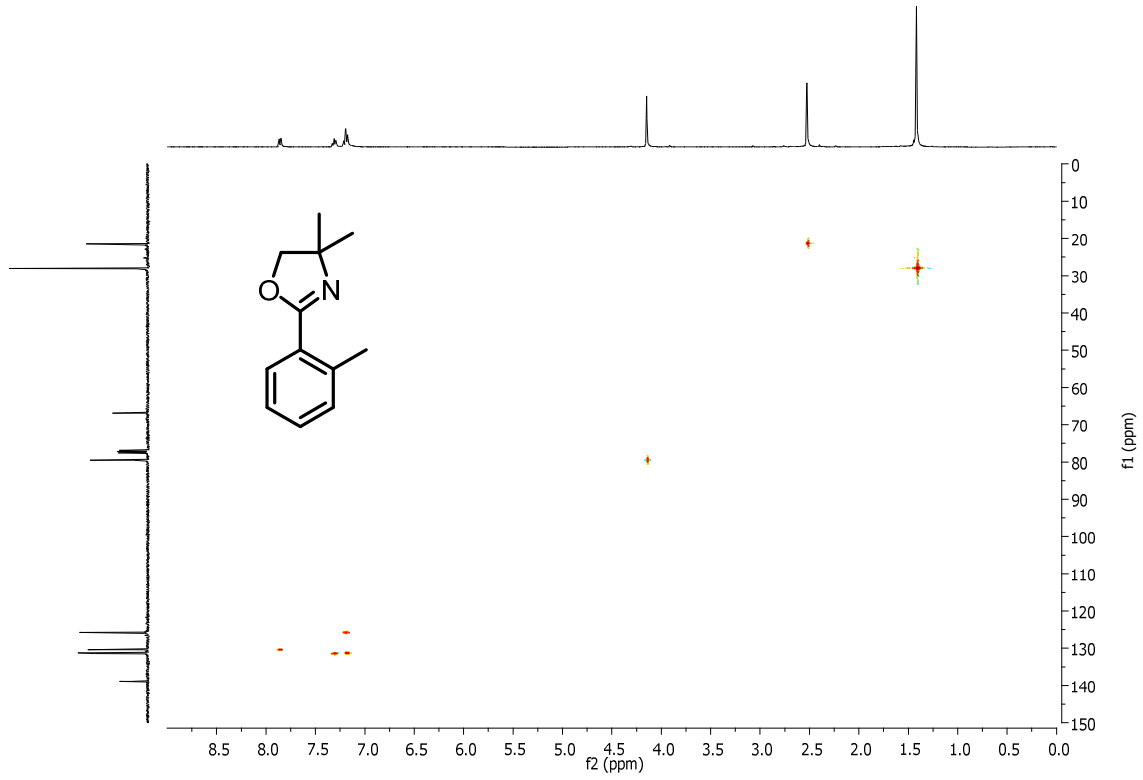


**Figure S34:** HSQC spectrum of **8** in $CDCl_3$*.

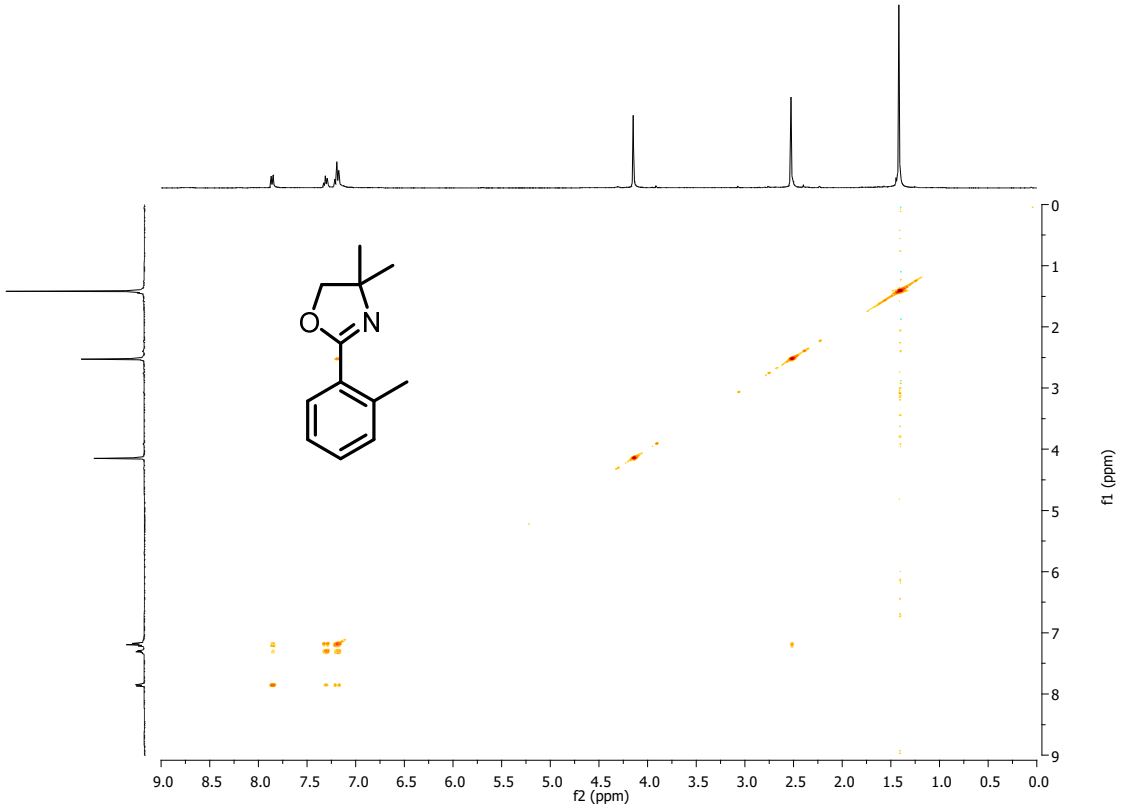


**Figure S35:** COSY spectrum of **8** in $CDCl_3$*.

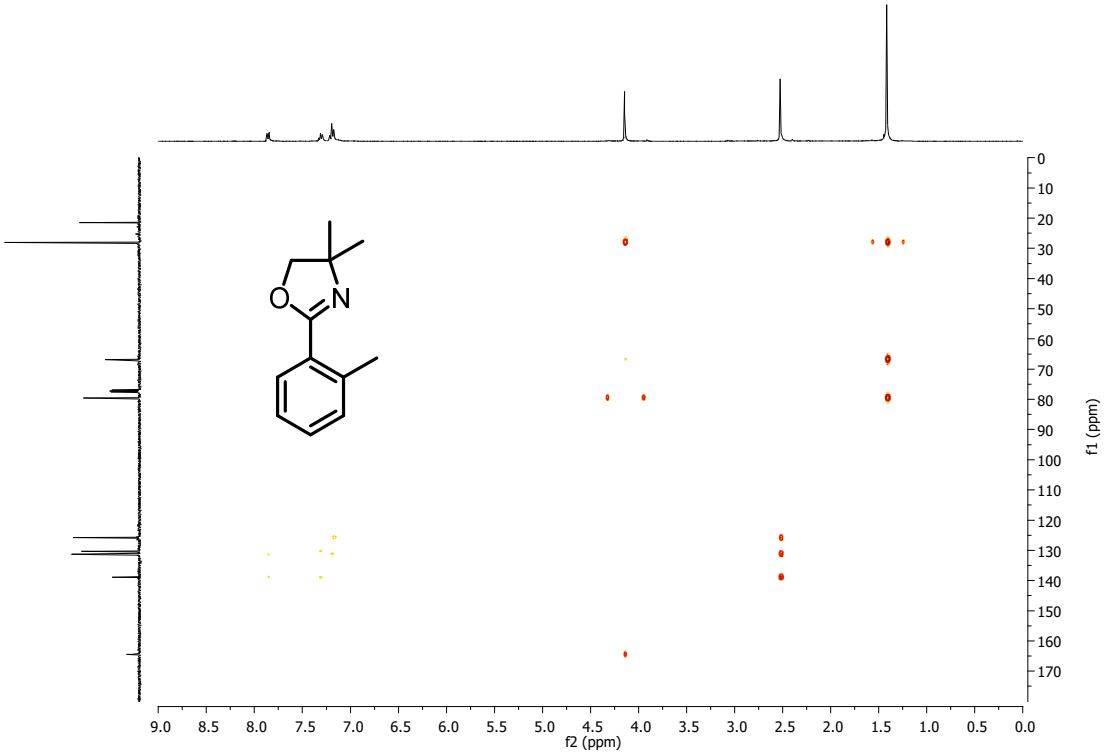


**Figure S36:** HMBC spectrum of **8** in $CDCl_3$*.

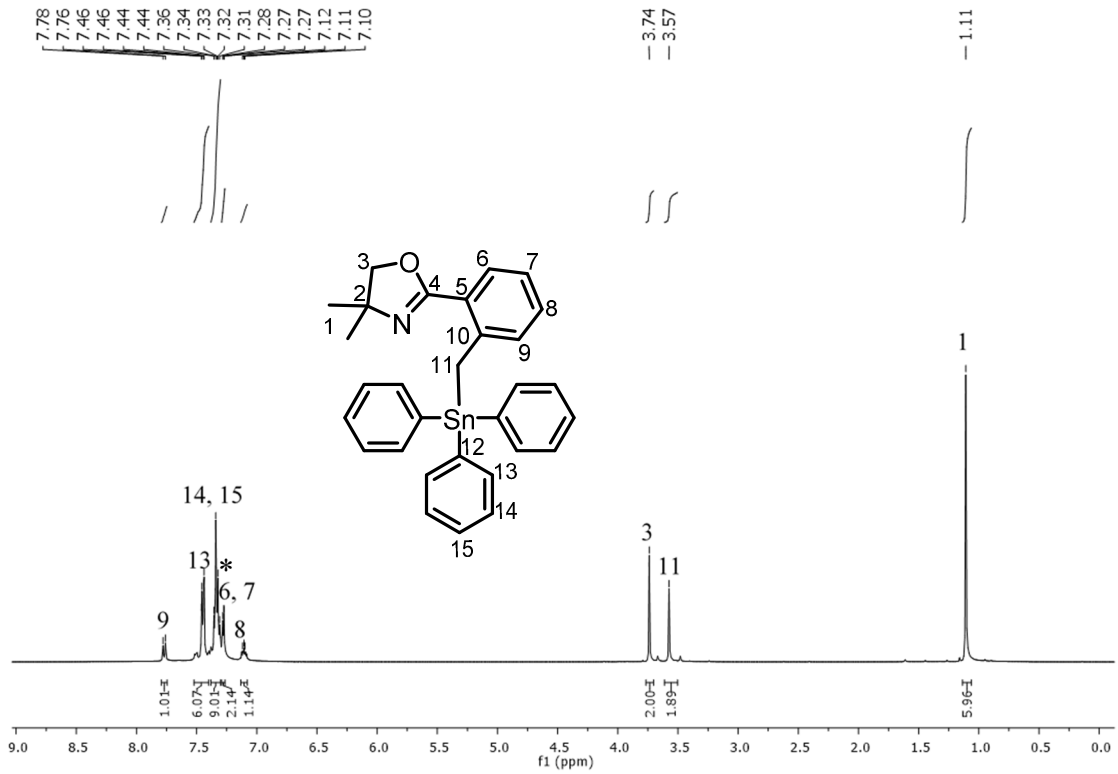


**Figure S37:** $^{1}$H NMR spectrum of **4** in $CDCl_3$*.

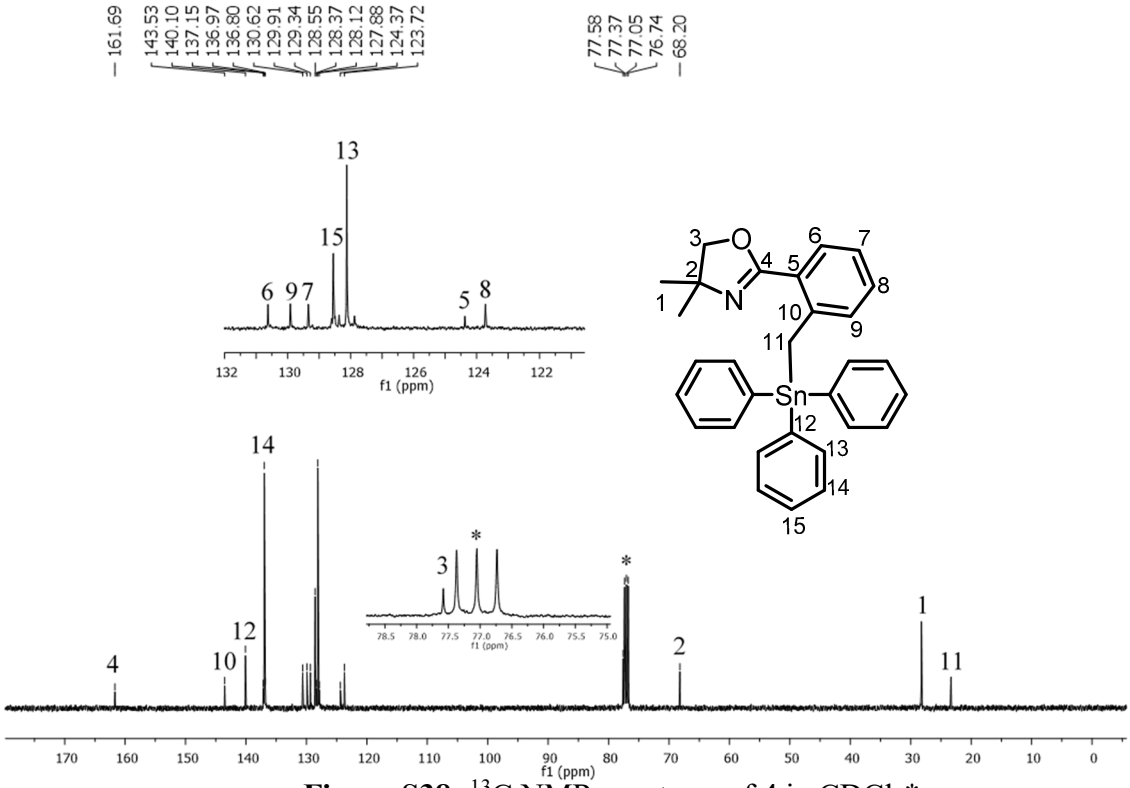


**Figure S38:** $^{13}$C NMR spectrum of **4** in $CDCl_3$*.

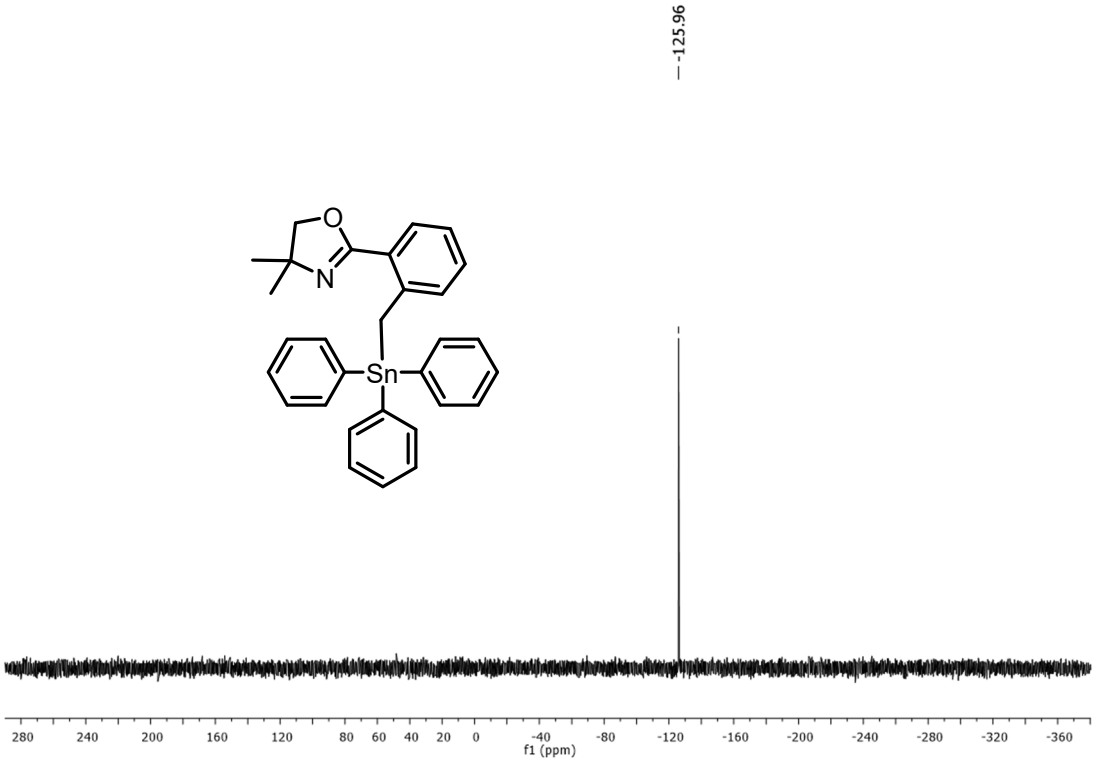


**Figure S39:** $^{119}$Sn NMR spectrum of **4** in $CDCl_3$.

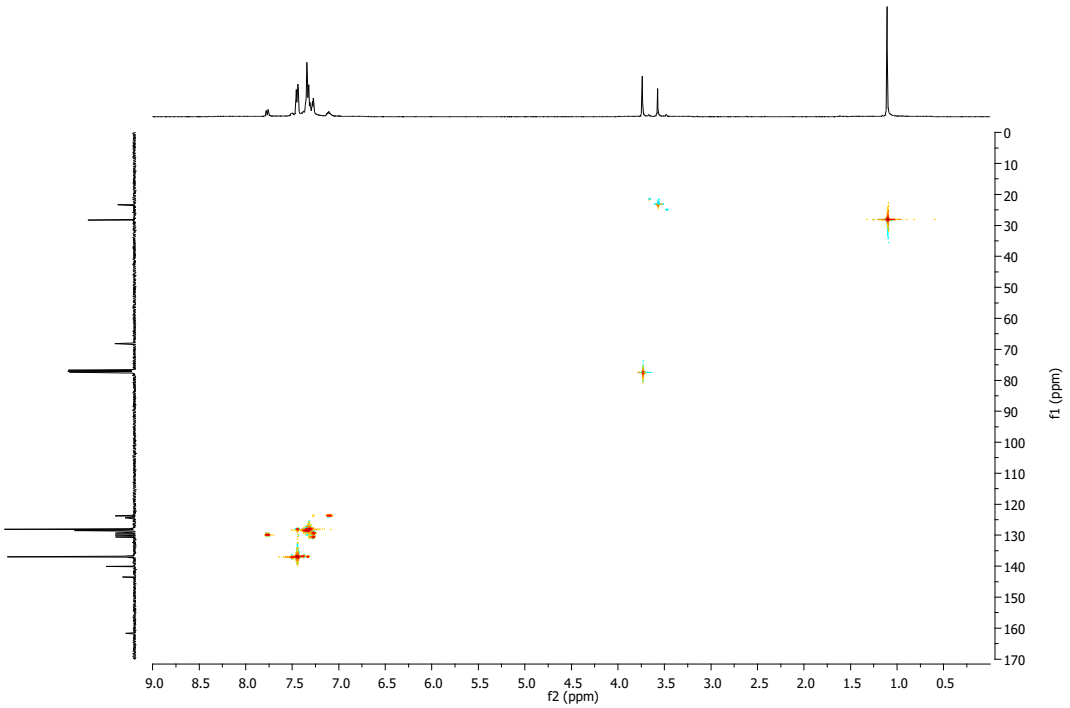


**Figure S40:** HSQC spectrum of **4** in $CDCl_3$.

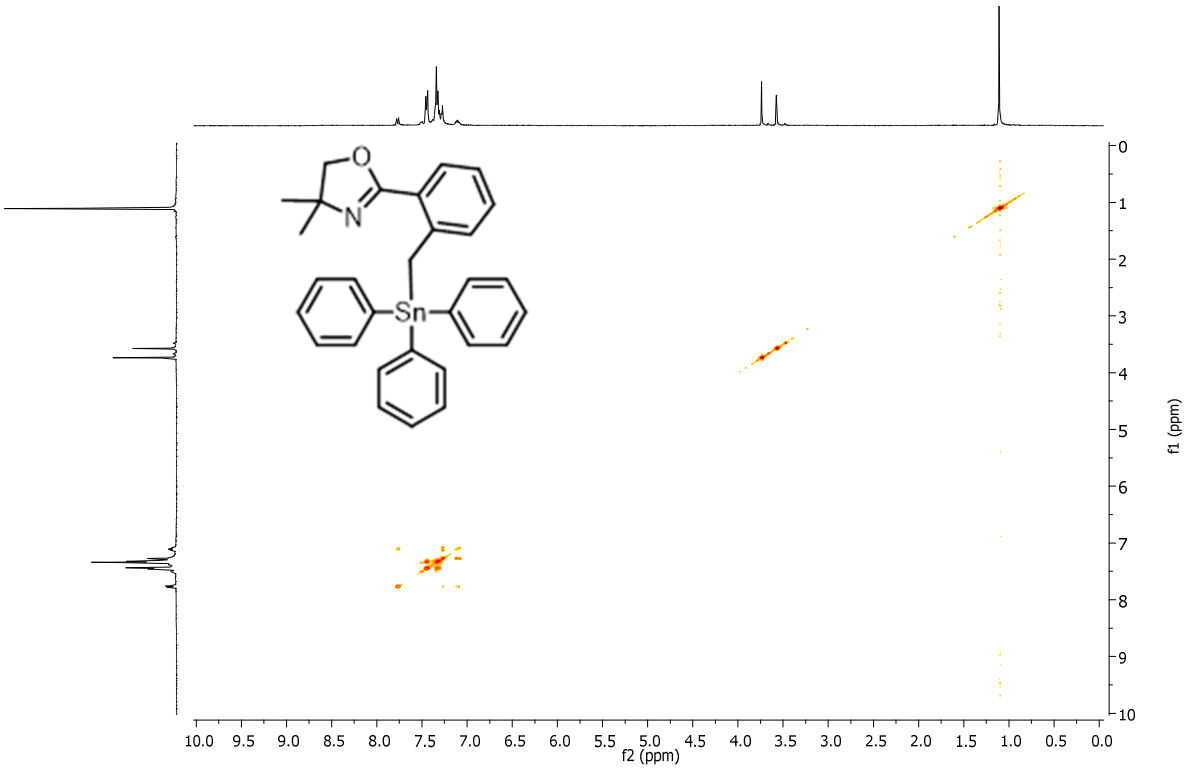


**Figure S41:** COSY spectrum of **4** in $CDCl_3$.

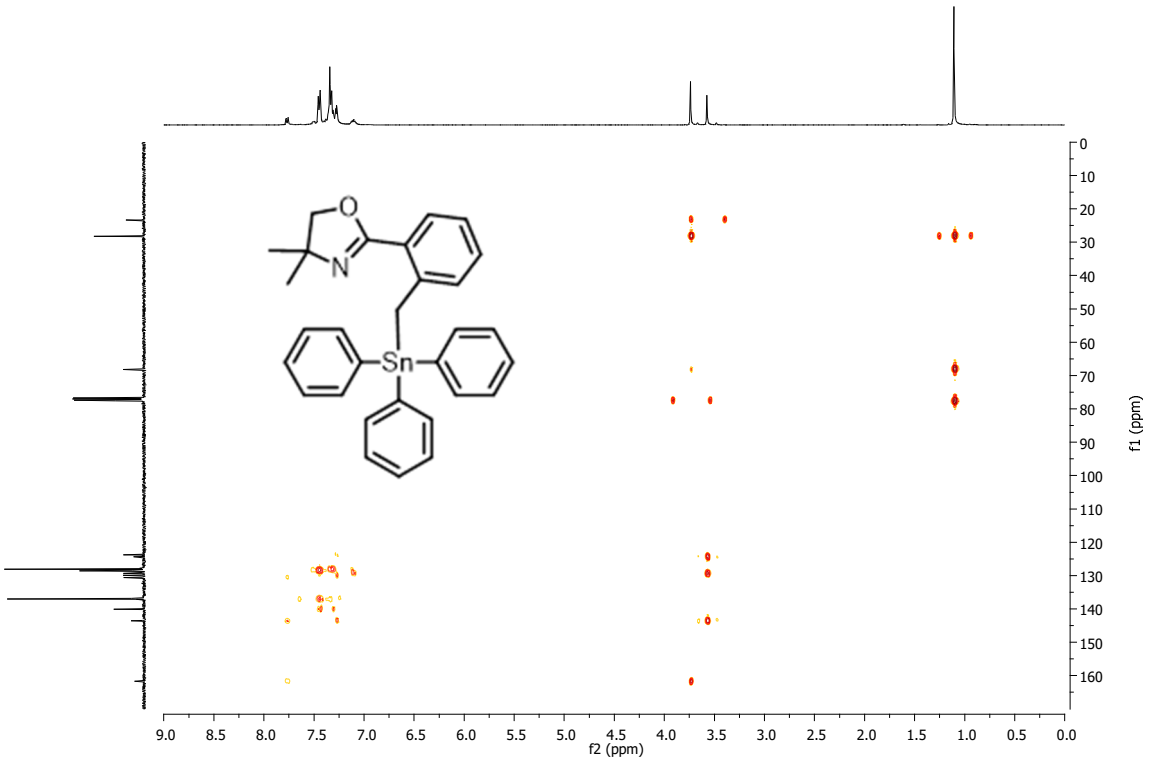


**Figure S42:** HMBC spectrum of **4** in $CDCl_3$.

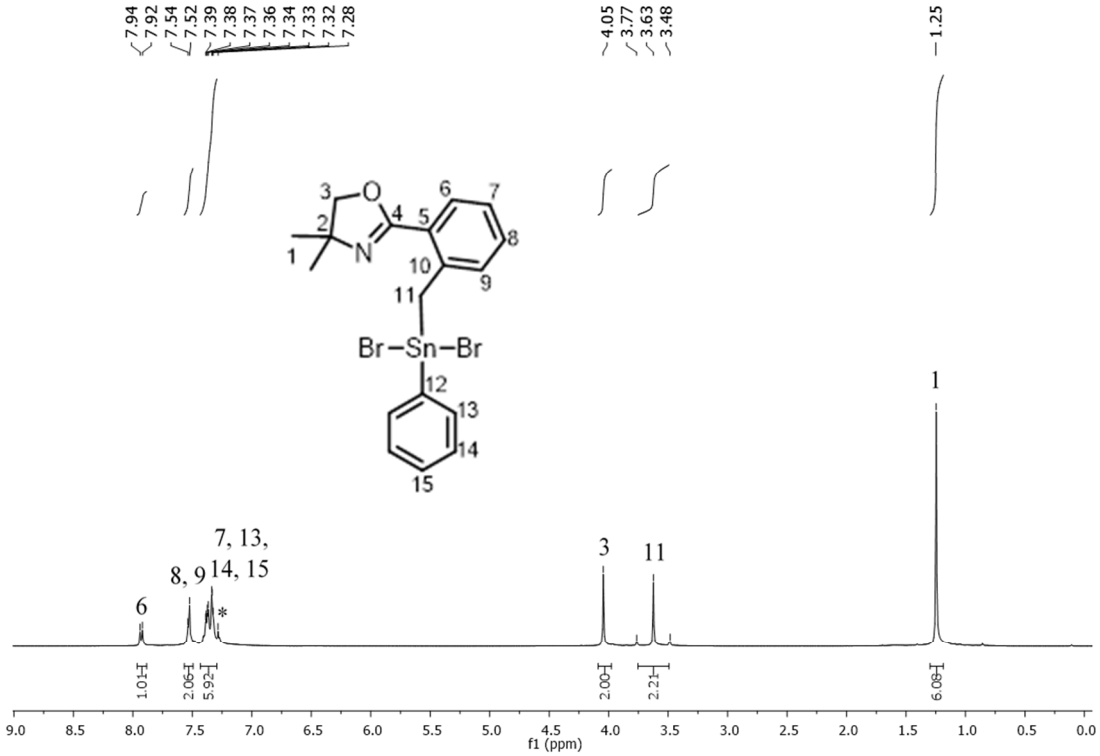


**Figure S43:** $^{1}$H NMR spectrum of **11** in $CDCl_3$*.

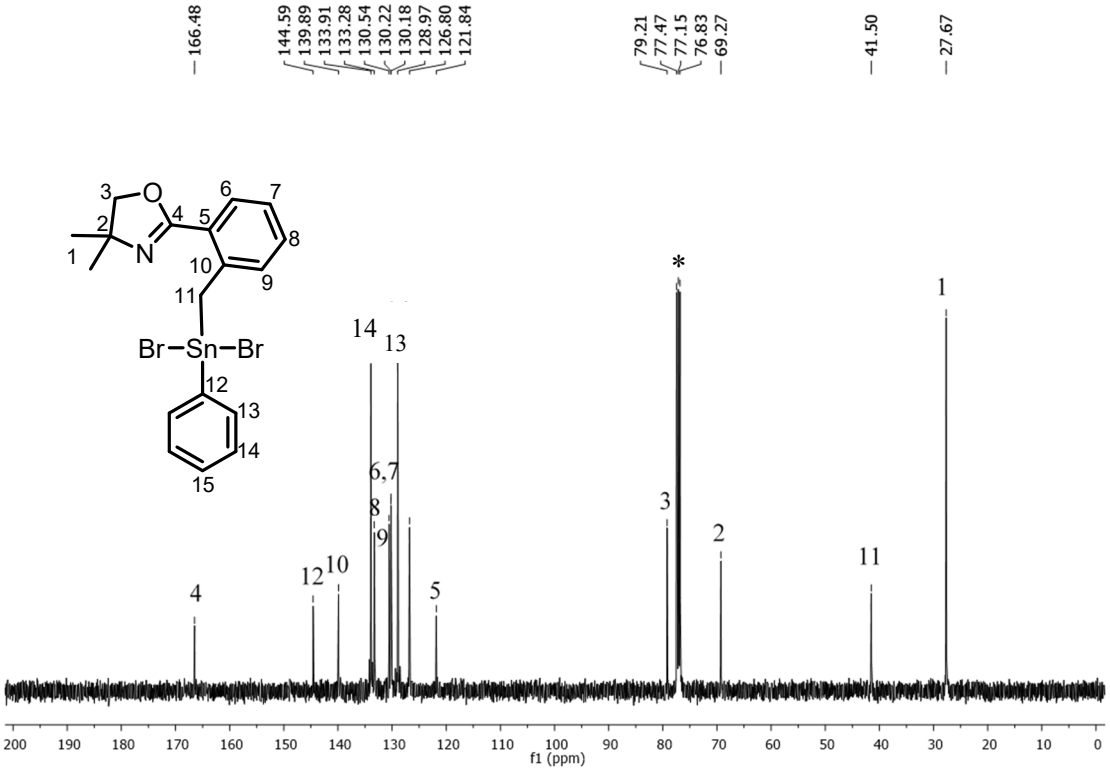


**Figure S44:** $^{13}$C NMR spectrum of **11** in $CDCl_3$*.

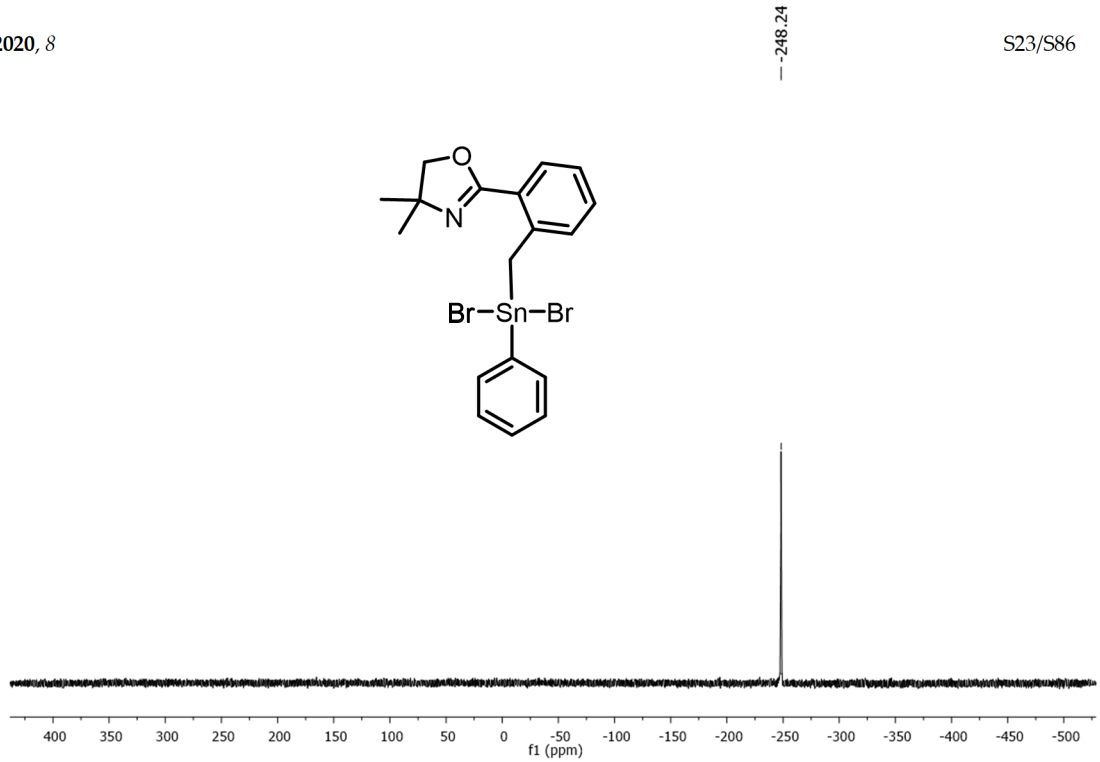


**Figure S45:** $^{119}$Sn NMR spectrum of **11** in $CDCl_3$.

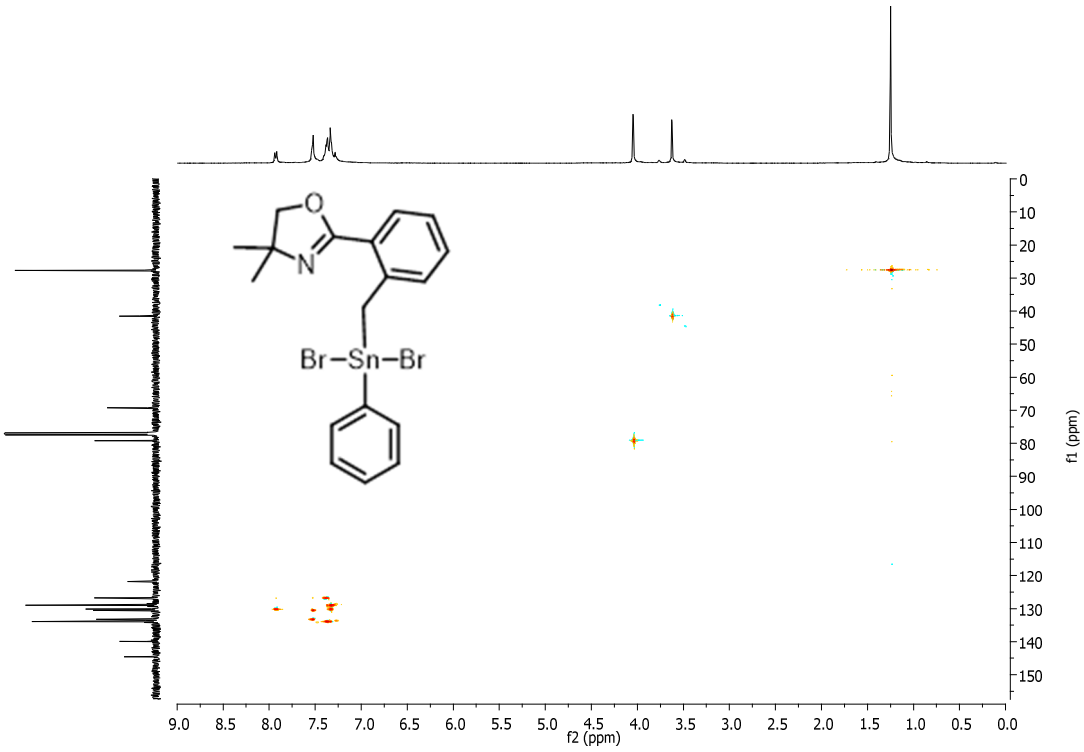


**Figure S46:** HSQC spectrum of **11** in $CDCl_3$.

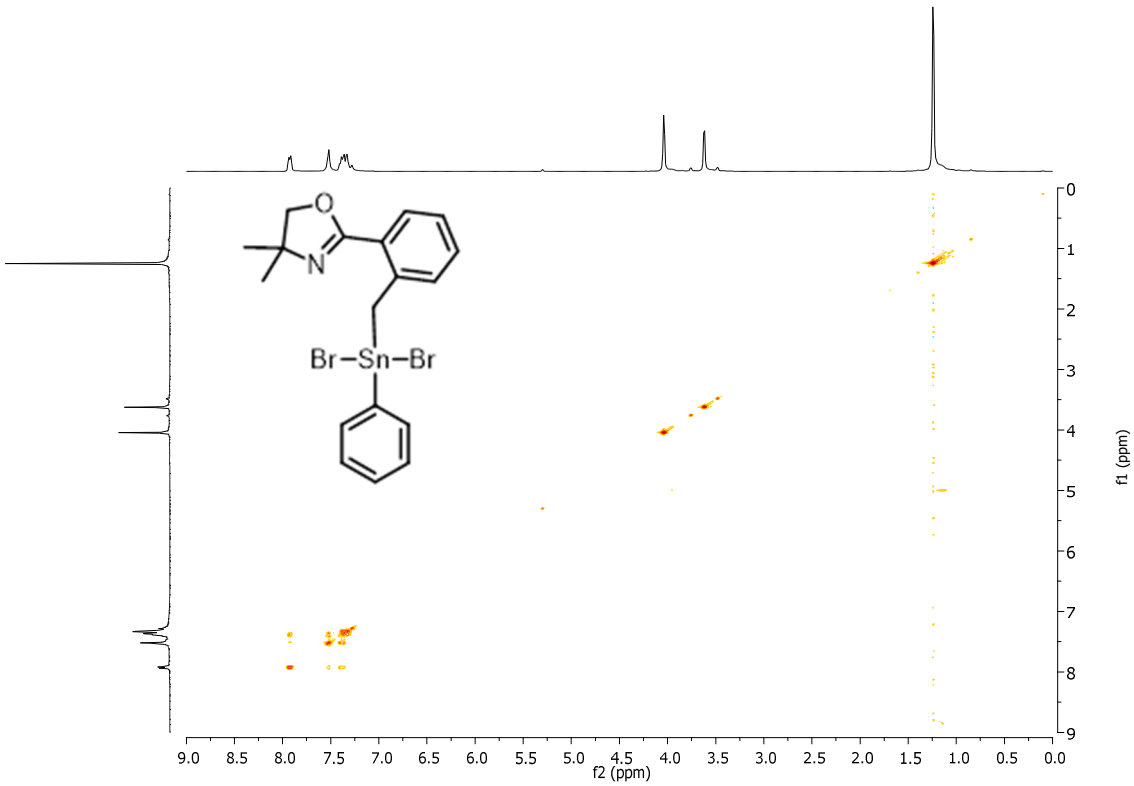


**Figure S47:** COSY spectrum of **11** in $CDCl_3$.

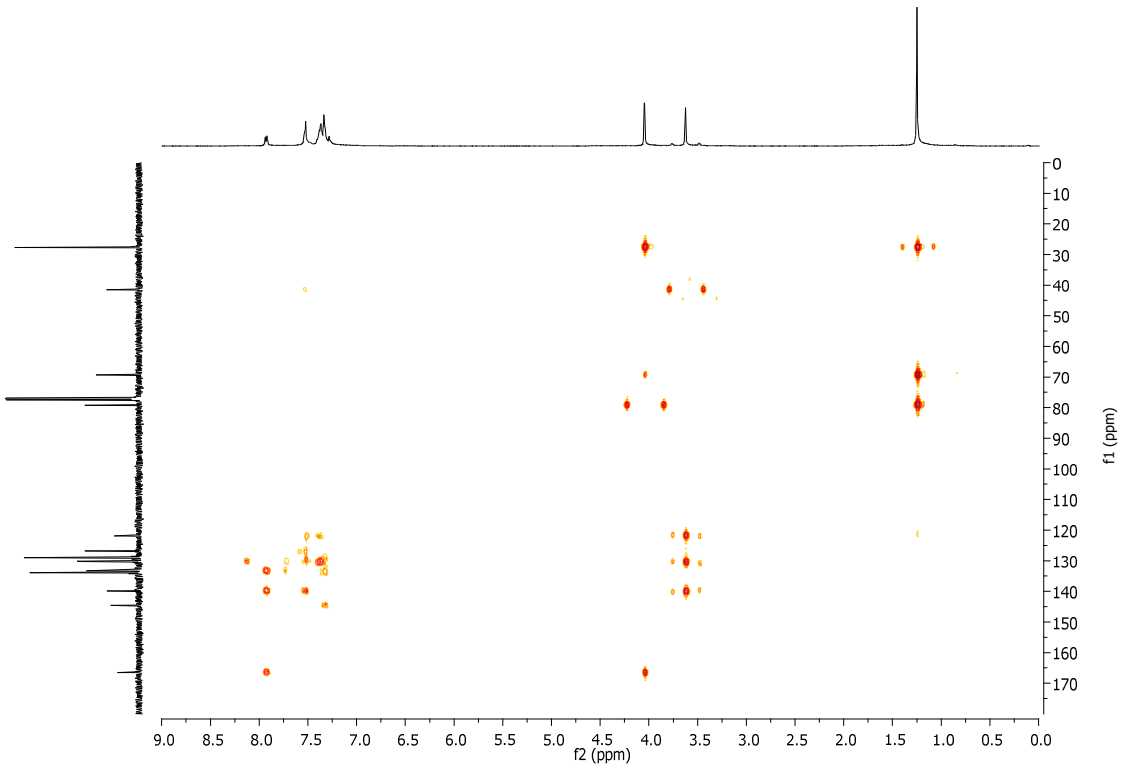


**Figure S48:** HMBC spectrum of **11** in $CDCl_3$.

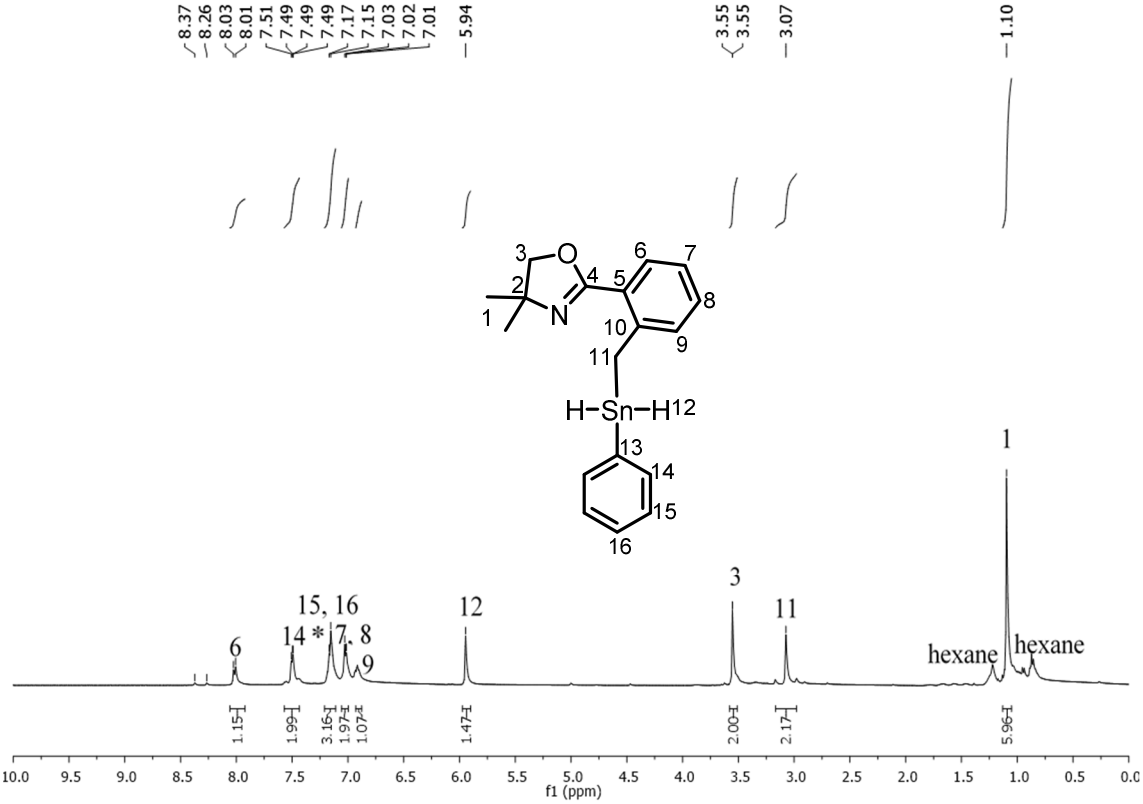


**Figure S49:** $^{1}$H NMR spectrum of **13** in $C_6D_6$*.

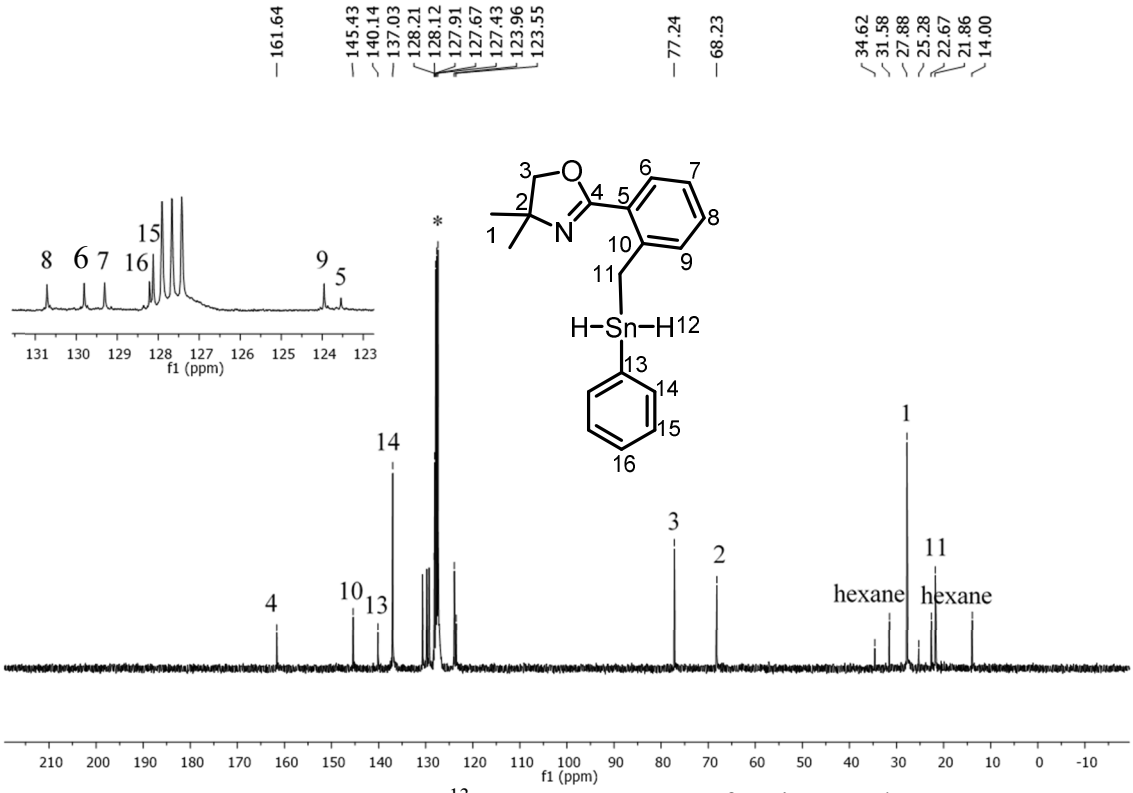


**Figure S50:** $^{13}$C NMR spectrum of **13** in $C_6D_6$*.

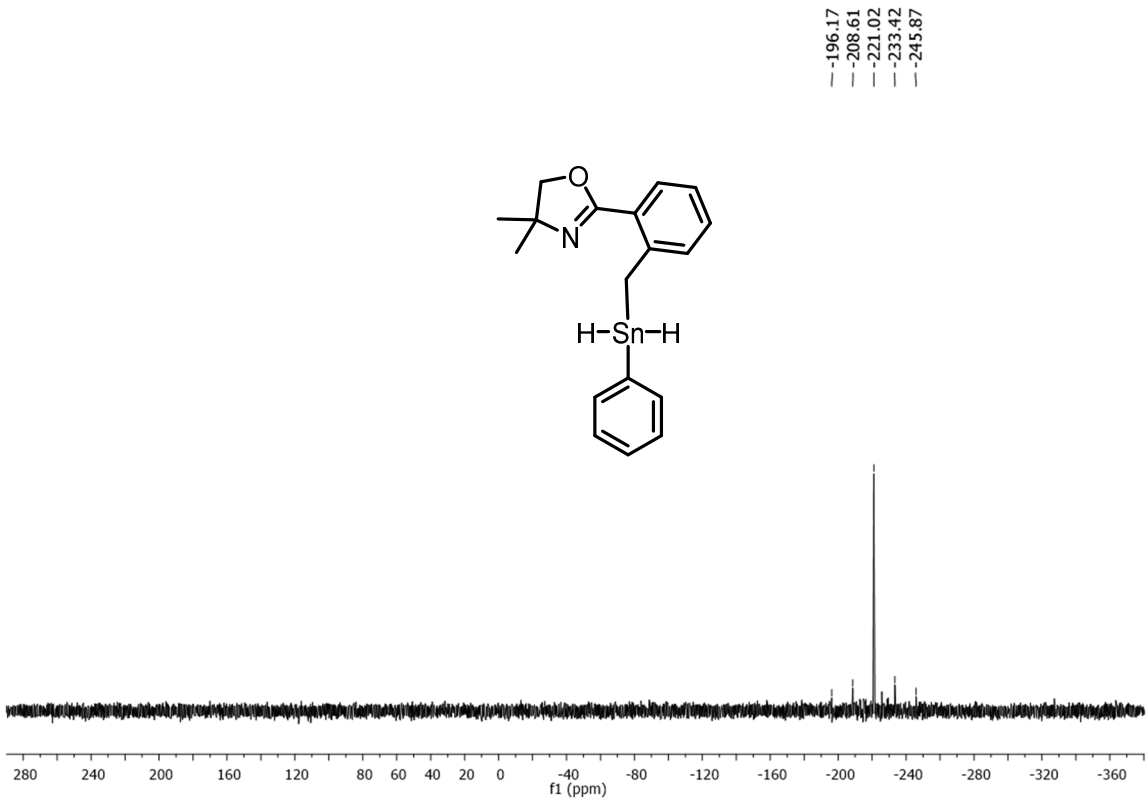


**Figure S51:** $^{119}$Sn NMR spectrum of **13** in $C_6D_6$.

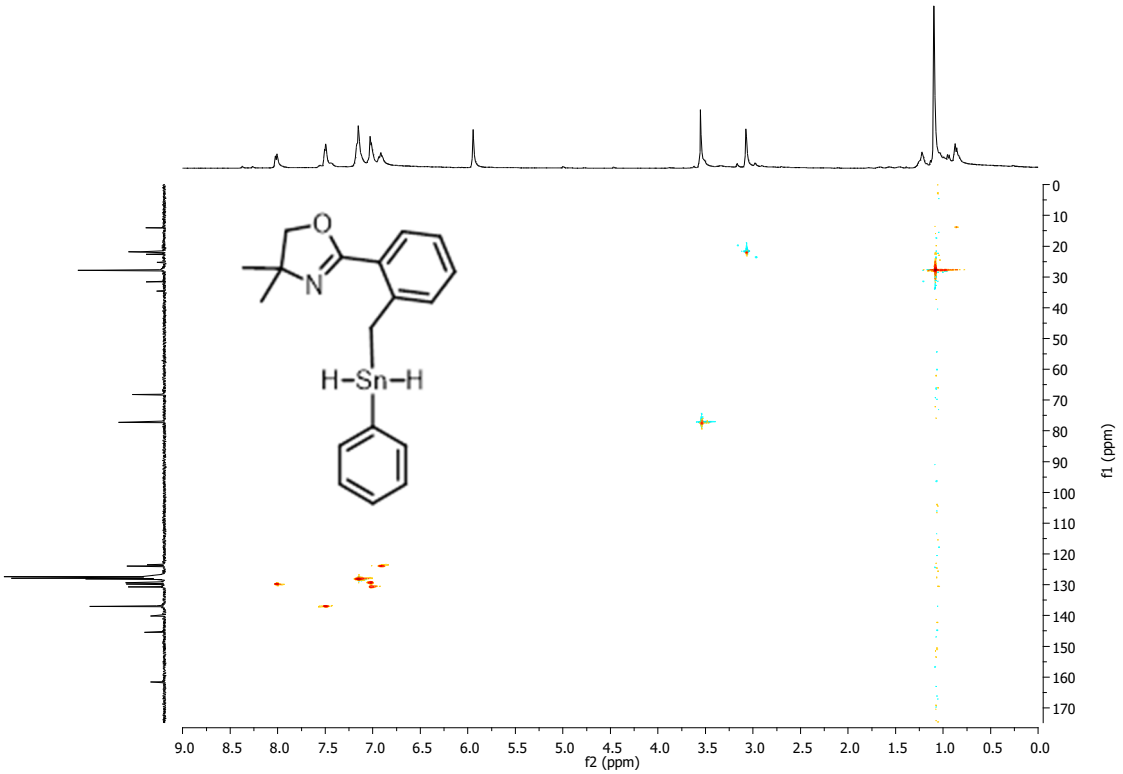


**Figure S52:** HSQC spectrum of **13** in $C_6D_6$.

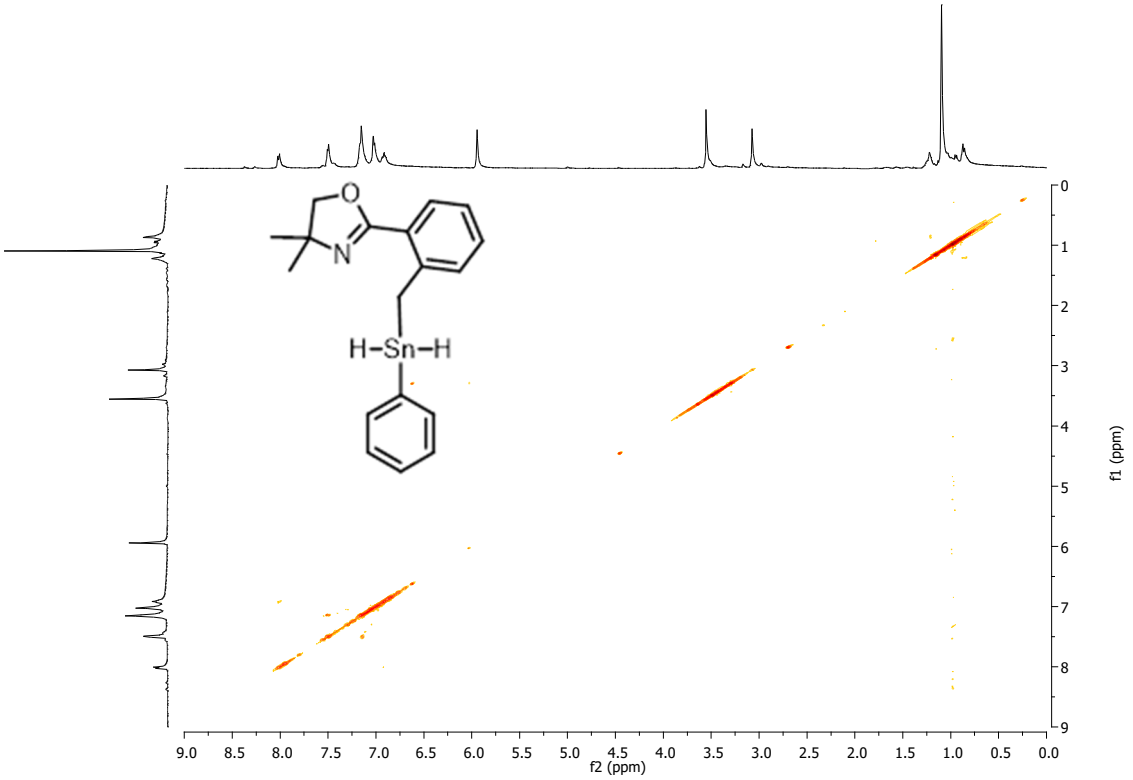


**Figure S53:** COSY spectrum of **13** in $C_6D_6$.

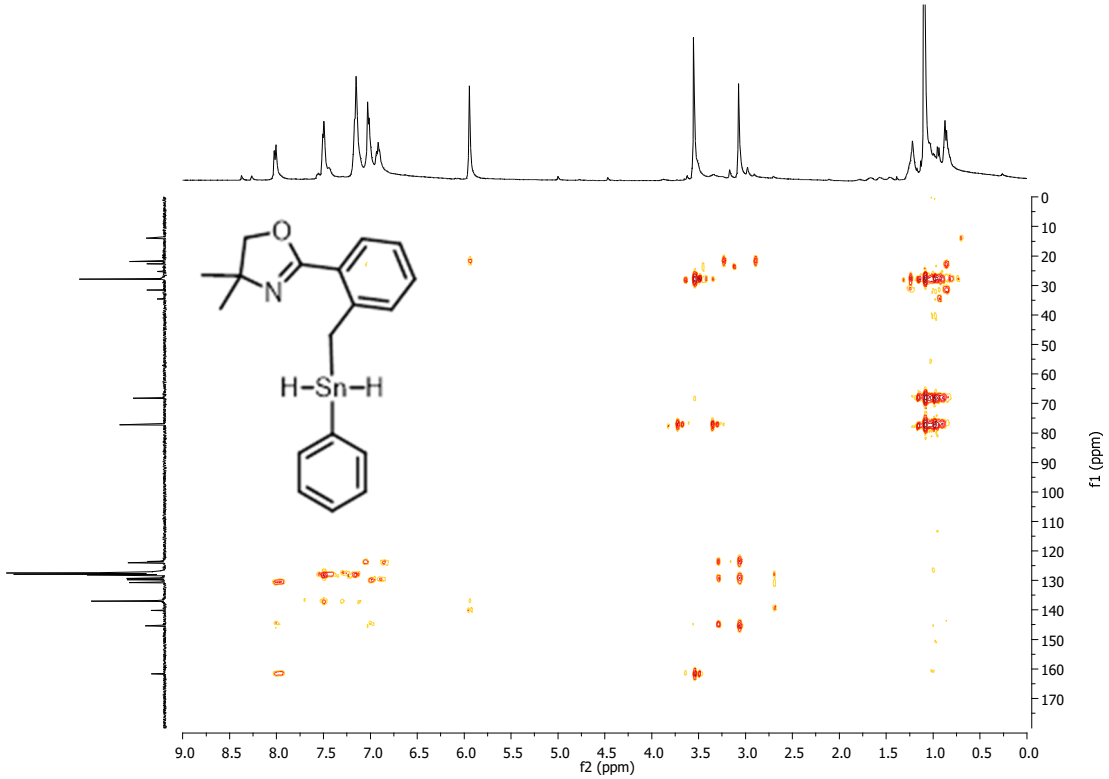


**Figure S54:** HMBC spectrum of **13** in $C_6D_6$.

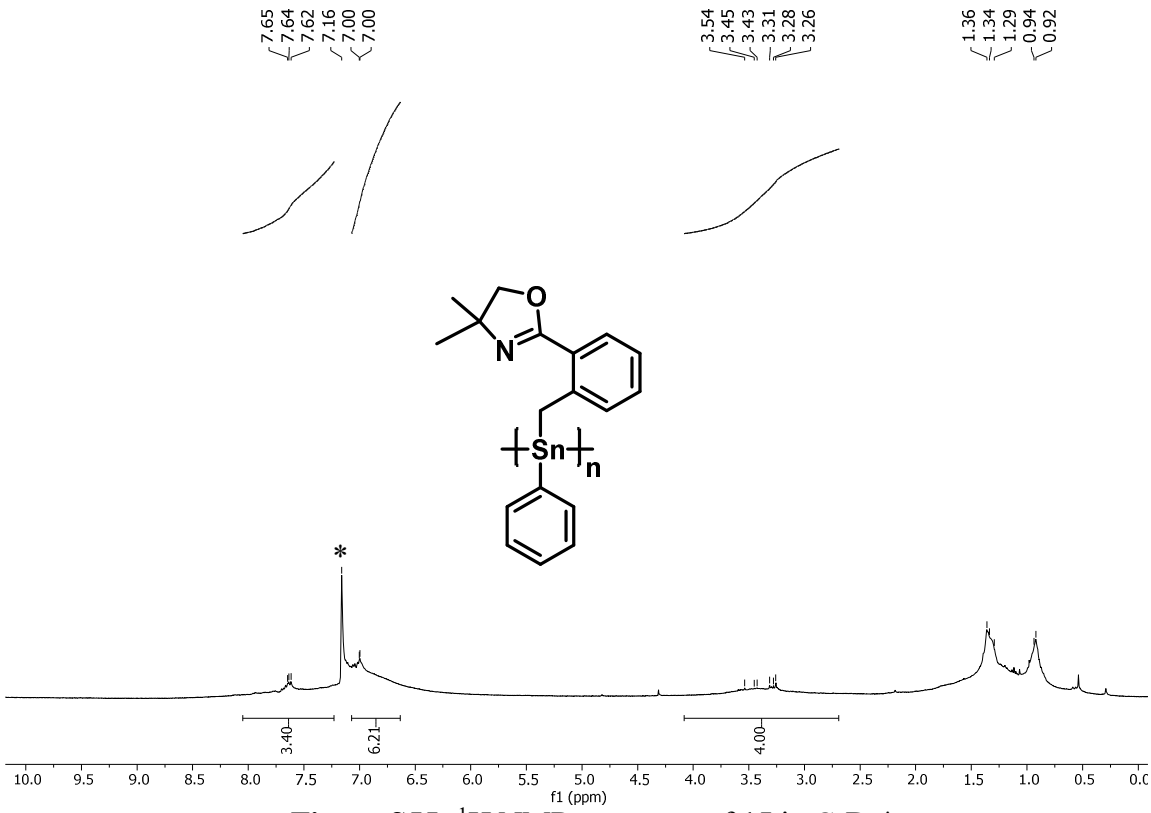


**Figure S55:** $^{1}$H NMR spectrum of **15** in $C_6D_6$*.

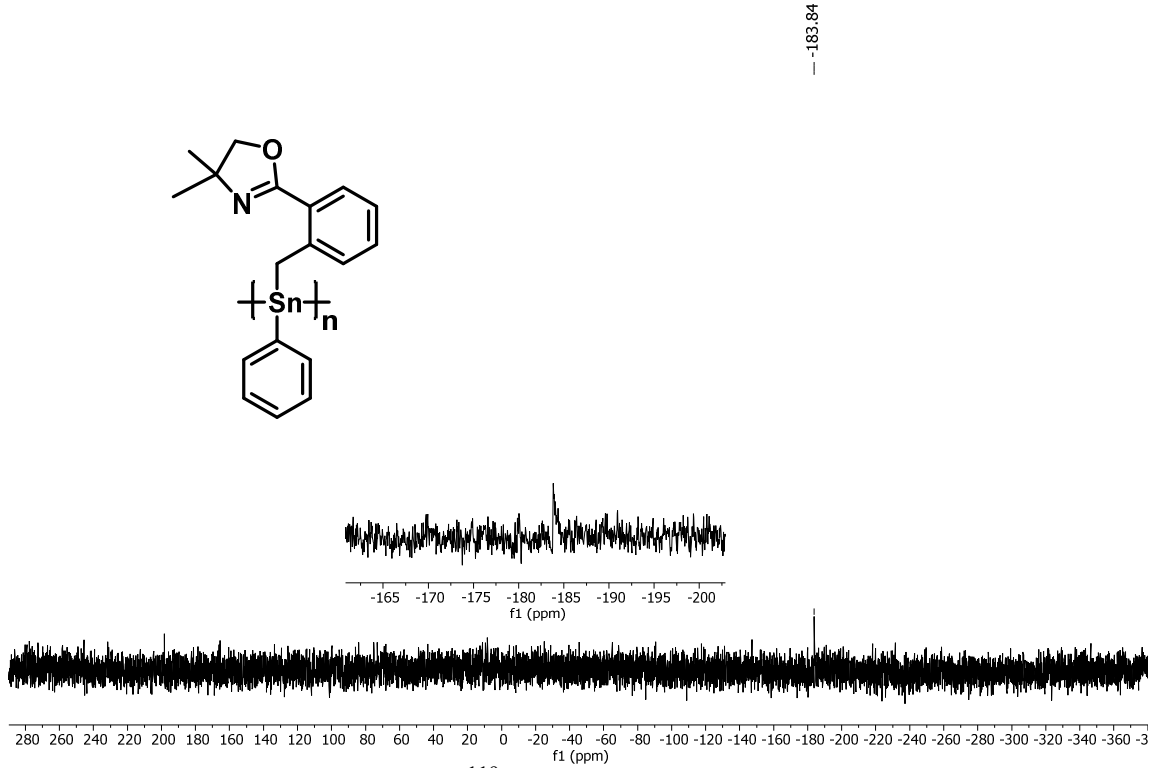


**Figure S56:** $^{119}$Sn NMR spectrum of **15** in $C_6D_6$.

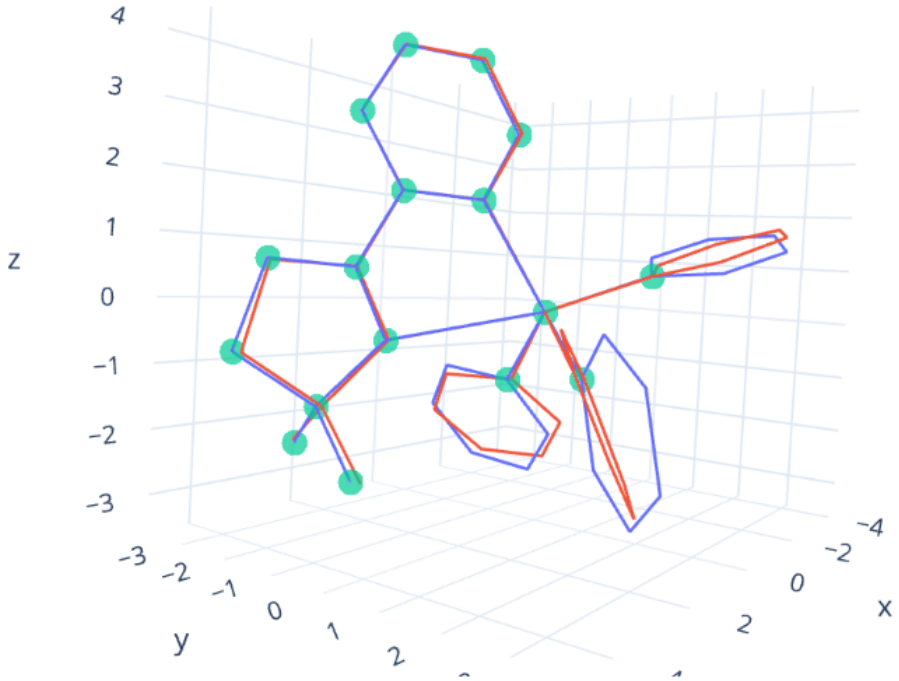


**Figure S57:** Overlay of coordinate traces for experimental (blue) and PBE0-GD3BJ (red) data for Compound **7**. Green points are coordinates used in calculation and minimization of MSSD.

**Table S1**. B3PW91-GD3BJ calculated bond lengths and differences for Compound **4'**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1A | C25A | 2.1357 | 0.0074 |
| Sn1A | C19A | 2.1343 | 0.0155 |
| Sn1A | C13A | 2.1571 | 0.0012 |
| Sn1A | C1A | 2.1631 | -0.0011 |
| O1A | C8A | 1.3600 | 0.0075 |
| O1A | C9A | 1.4403 | 0.0003 |
| N1A | C8A | 1.2832 | -0.0088 |
| N1A | C10A | 1.4765 | 0.0076 |
| C1A | C2A | 1.4863 | 0.0048 |
| C2A | C3A | 1.4034 | -0.0068 |
| C2A | C7A | 1.4166 | 0.0012 |
| C3A | C4A | 1.3906 | -0.0226 |
| C4A | C5A | 1.3960 | 0.0045 |
| C5A | C6A | 1.3886 | -0.0051 |
| C6A | C7A | 1.4040 | -0.0117 |
| C7A | C8A | 1.4644 | 0.0082 |
| C9A | C10A | 1.5509 | -0.0191 |
| C10A | C11A | 1.5257 | -0.0073 |
| C10A | C12A | 1.5294 | -0.0070 |
| C13A | C18A | 1.4025 | -0.0104 |
| C13A | C14A | 1.4031 | -0.0069 |
| C14A | C15A | 1.3960 | -0.0160 |
| C15A | C16A | 1.3958 | -0.0206 |
| C16A | C17A | 1.3954 | -0.0318 |
| C17A | C18A | 1.3966 | -0.0025 |
| C19A | C20A | 1.4019 | -0.0189 |
| C19A | C24A | 1.4016 | -0.0063 |
| C20A | C21A | 1.3959 | -0.0130 |
| C21A | C22A | 1.3953 | -0.0184 |
| C22A | C23A | 1.3955 | -0.0132 |
| C23A | C24A | 1.3960 | -0.0034 |
| C25A | C30A | 1.4013 | -0.0123 |
| C25A | C26A | 1.4035 | -0.0089 |
| C26A | C27A | 1.3960 | -0.0081 |
| C27A | C28A | 1.3948 | -0.0144 |
| C28A | C29A | 1.3954 | -0.0135 |
| C29A | C30A | 1.3954 | -0.0032 |
| Sn1A | N1A | 2.8175 | 0.3581 |

**Table S2**. B3PW91-GD3BJ calculated bond angles and differences for Compound **4'**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C25A | Sn1A | C19A | 114.0 | -3.7 |
| C25A | Sn1A | C13A | 100.7 | 4.1 |
| C19A | Sn1A | C13A | 102.9 | 5.4 |
| C25A | Sn1A | C1A | 121.0 | -5.5 |
| C19A | Sn1A | C1A | 110.7 | 2.8 |
| C13A | Sn1A | C1A | 104.8 | -1.2 |
| C8A | O1A | C9A | 106.3 | -1.1 |
| C8A | N1A | C10A | 108.0 | -1.0 |
| C2A | C1A | Sn1A | 114.1 | -4.2 |
| C3A | C2A | C7A | 117.3 | -0.3 |
| C3A | C2A | C1A | 119.4 | -0.2 |
| C7A | C2A | C1A | 123.3 | 0.5 |
| C4A | C3A | C2A | 122.0 | 0.9 |
| C3A | C4A | C5A | 120.1 | -0.3 |
| C6A | C5A | C4A | 119.2 | -0.5 |
| C5A | C6A | C7A | 120.9 | 0.7 |
| C6A | C7A | C2A | 120.4 | -0.5 |
| C6A | C7A | C8A | 118.1 | 0.6 |
| C2A | C7A | C8A | 121.4 | -0.1 |
| N1A | C8A | O1A | 117.1 | 0.4 |
| N1A | C8A | C7A | 126.7 | 0.9 |
| O1A | C8A | C7A | 116.0 | -1.2 |
| O1A | C9A | C10A | 104.7 | -0.2 |
| N1A | C10A | C11A | 110.6 | -1.8 |
| N1A | C10A | C12A | 108.9 | 0.1 |
| C11A | C10A | C12A | 110.9 | 0.1 |
| N1A | C10A | C9A | 102.7 | 0.3 |
| C11A | C10A | C9A | 111.8 | 0.6 |
| C12A | C10A | C9A | 111.6 | 0.7 |
| C18A | C13A | C14A | 118.0 | -0.1 |
| C18A | C13A | Sn1A | 121.2 | 0.3 |
| C14A | C13A | Sn1A | 120.8 | -0.2 |
| C15A | C14A | C13A | 121.2 | 0.2 |
| C16A | C15A | C14A | 120.0 | -0.1 |
| C17A | C16A | C15A | 119.7 | 0.3 |
| C16A | C17A | C18A | 120.0 | 0.9 |
| C13A | C18A | C17A | 121.2 | -1.1 |
| C20A | C19A | C24A | 118.1 | 0.1 |
| C20A | C19A | Sn1A | 120.3 | 2.1 |
| C24A | C19A | Sn1A | 121.6 | -2.2 |
| C21A | C20A | C19A | 121.2 | -0.3 |
| C22A | C21A | C20A | 120.0 | 0.7 |
| C21A | C22A | C23A | 119.7 | -0.1 |
| C22A | C23A | C24A | 120.0 | -0.3 |
| C23A | C24A | C19A | 121.1 | -0.2 |

| | | | | |
|---|---|---|---|---|
| C30A | C25A | C26A | 118.1 | -0.3 |
| C30A | C25A | Sn1A | 125.5 | -3.1 |
| C26A | C25A | Sn1A | 116.4 | 3.4 |
| C27A | C26A | C25A | 121.2 | 0.0 |
| C28A | C27A | C26A | 119.9 | 0.2 |
| C27A | C28A | C29A | 119.6 | 0.0 |
| C28A | C29A | C30A | 120.2 | -0.1 |
| C25A | C30A | C29A | 121.0 | 0.2 |

**Table S3**. PBE0-GD3BJ calculated bond lengths and differences for Compound **4'**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1A | C25A | 2.1409 | 0.002 |
| Sn1A | C19A | 2.1391 | 0.011 |
| Sn1A | C13A | 2.1614 | -0.003 |
| Sn1A | C1A | 2.1656 | -0.004 |
| O1A | C8A | 1.3563 | 0.011 |
| O1A | C9A | 1.4351 | 0.006 |
| N1A | C8A | 1.2813 | -0.007 |
| N1A | C10A | 1.4735 | 0.011 |
| C1A | C2A | 1.4857 | 0.005 |
| C2A | C3A | 1.4024 | -0.006 |
| C2A | C7A | 1.4147 | 0.003 |
| C3A | C4A | 1.3894 | -0.021 |
| C4A | C5A | 1.3946 | 0.006 |
| C5A | C6A | 1.3875 | -0.004 |
| C6A | C7A | 1.4026 | -0.010 |
| C7A | C8A | 1.4646 | 0.008 |
| C9A | C10A | 1.5484 | -0.017 |
| C10A | C11A | 1.5242 | -0.006 |
| C10A | C12A | 1.5276 | -0.005 |
| C13A | C18A | 1.4015 | -0.009 |
| C13A | C14A | 1.4022 | -0.006 |
| C14A | C15A | 1.3948 | -0.015 |
| C15A | C16A | 1.3944 | -0.019 |
| C16A | C17A | 1.3938 | -0.030 |
| C17A | C18A | 1.3955 | -0.001 |
| C19A | C20A | 1.4010 | -0.018 |
| C19A | C24A | 1.4008 | -0.005 |
| C20A | C21A | 1.3949 | -0.012 |
| C21A | C22A | 1.3939 | -0.017 |
| C22A | C23A | 1.3941 | -0.012 |
| C23A | C24A | 1.3950 | -0.002 |
| C25A | C30A | 1.4004 | -0.011 |
| C25A | C26A | 1.4026 | -0.008 |
| C26A | C27A | 1.3950 | -0.007 |
| C27A | C28A | 1.3933 | -0.013 |
| C28A | C29A | 1.3940 | -0.012 |
| C29A | C30A | 1.3944 | -0.002 |
| Sn1A | N1A | 2.8619 | 0.314 |

**Table S4.** PBE0-GD3BJ calculated bond angles and differences for Compound **4'**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C25A | Sn1A | C19A | 114.0 | -3.4 |
| C25A | Sn1A | C13A | 100.7 | 3.8 |
| C19A | Sn1A | C13A | 102.9 | 5.2 |
| C25A | Sn1A | C1A | 121.0 | -5.7 |
| C19A | Sn1A | C1A | 110.7 | 2.8 |
| C13A | Sn1A | C1A | 104.8 | -0.8 |
| C8A | O1A | C9A | 106.3 | -1.1 |
| C8A | N1A | C10A | 108.0 | -0.8 |
| C2A | C1A | Sn1A | 114.1 | -4.9 |
| C3A | C2A | C7A | 117.3 | -0.3 |
| C3A | C2A | C1A | 119.4 | -0.2 |
| C7A | C2A | C1A | 123.3 | 0.4 |
| C4A | C3A | C2A | 122.0 | 0.9 |
| C3A | C4A | C5A | 120.1 | -0.3 |
| C6A | C5A | C4A | 119.2 | -0.5 |
| C5A | C6A | C7A | 120.9 | 0.6 |
| C6A | C7A | C2A | 120.4 | -0.5 |
| C6A | C7A | C8A | 118.1 | 0.6 |
| C2A | C7A | C8A | 121.4 | -0.1 |
| N1A | C8A | O1A | 117.1 | 0.2 |
| N1A | C8A | C7A | 126.7 | 0.9 |
| O1A | C8A | C7A | 116.0 | -1.0 |
| O1A | C9A | C10A | 104.7 | -0.2 |
| N1A | C10A | C11A | 110.6 | -1.8 |
| N1A | C10A | C12A | 108.9 | -0.1 |
| C11A | C10A | C12A | 110.9 | 0.2 |
| N1A | C10A | C9A | 102.7 | 0.2 |
| C11A | C10A | C9A | 111.8 | 0.7 |
| C12A | C10A | C9A | 111.6 | 0.7 |
| C18A | C13A | C14A | 118.0 | 0.0 |
| C18A | C13A | Sn1A | 121.2 | 0.2 |
| C14A | C13A | Sn1A | 120.8 | -0.2 |
| C15A | C14A | C13A | 121.2 | 0.1 |
| C16A | C15A | C14A | 120.0 | -0.1 |
| C17A | C16A | C15A | 119.7 | 0.3 |
| C16A | C17A | C18A | 120.0 | 0.9 |
| C13A | C18A | C17A | 121.2 | -1.2 |
| C20A | C19A | C24A | 118.1 | 0.2 |
| C20A | C19A | Sn1A | 120.3 | 2.0 |
| C24A | C19A | Sn1A | 121.6 | -2.1 |
| C21A | C20A | C19A | 121.2 | -0.3 |
| C22A | C21A | C20A | 120.0 | 0.7 |
| C21A | C22A | C23A | 119.7 | -0.1 |
| C22A | C23A | C24A | 120.0 | -0.3 |
| C23A | C24A | C19A | 121.1 | -0.2 |

| | | | | |
|---|---|---|---|---|
| C30A | C25A | C26A | 118.1 | -0.3 |
| C30A | C25A | Sn1A | 125.5 | -3.2 |
| C26A | C25A | Sn1A | 116.4 | 3.5 |
| C27A | C26A | C25A | 121.2 | 0.0 |
| C28A | C27A | C26A | 119.9 | 0.2 |
| C27A | C28A | C29A | 119.6 | 0.0 |
| C28A | C29A | C30A | 120.2 | -0.1 |
| C25A | C30A | C29A | 121.0 | 0.2 |

**Table S5**. M05-2X-GD3 calculated bond lengths and differences for Compound **4'**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1A | C25A | 2.1335 | 0.010 |
| Sn1A | C19A | 2.1306 | 0.019 |
| Sn1A | C13A | 2.1506 | 0.008 |
| Sn1A | C1A | 2.1576 | 0.004 |
| O1A | C8A | 1.3614 | 0.006 |
| O1A | C9A | 1.4416 | -0.001 |
| N1A | C8A | 1.2764 | -0.002 |
| N1A | C10A | 1.4770 | 0.007 |
| C1A | C2A | 1.4918 | -0.001 |
| C2A | C3A | 1.4022 | -0.006 |
| C2A | C7A | 1.4114 | 0.006 |
| C3A | C4A | 1.3893 | -0.021 |
| C4A | C5A | 1.3944 | 0.006 |
| C5A | C6A | 1.3877 | -0.004 |
| C6A | C7A | 1.4011 | -0.009 |
| C7A | C8A | 1.4701 | 0.003 |
| C9A | C10A | 1.5444 | -0.013 |
| C10A | C11A | 1.5243 | -0.006 |
| C10A | C12A | 1.5296 | -0.007 |
| C13A | C18A | 1.4006 | -0.008 |
| C13A | C14A | 1.4023 | -0.006 |
| C14A | C15A | 1.3943 | -0.014 |
| C15A | C16A | 1.3944 | -0.019 |
| C16A | C17A | 1.3931 | -0.029 |
| C17A | C18A | 1.3958 | -0.002 |
| C19A | C20A | 1.4007 | -0.018 |
| C19A | C24A | 1.4004 | -0.005 |
| C20A | C21A | 1.3948 | -0.012 |
| C21A | C22A | 1.3940 | -0.017 |
| C22A | C23A | 1.3939 | -0.012 |
| C23A | C24A | 1.3953 | -0.003 |
| C25A | C30A | 1.4002 | -0.011 |
| C25A | C26A | 1.4027 | -0.008 |
| C26A | C27A | 1.3948 | -0.007 |
| C27A | C28A | 1.3929 | -0.013 |
| C28A | C29A | 1.3935 | -0.012 |
| C29A | C30A | 1.3943 | -0.002 |
| Sn1A | N1A | 2.9590 | 0.217 |

**Table S6.** M05-2X-GD3 calculated bond angles and differences for Compound **4'**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C25A | Sn1A | C19A | 112.5 | -2.1 |
| C25A | Sn1A | C13A | 101.7 | 3.1 |
| C19A | Sn1A | C13A | 104.1 | 4.2 |
| C25A | Sn1A | C1A | 120.5 | -5.0 |
| C19A | Sn1A | C1A | 111.3 | 2.2 |
| C13A | Sn1A | C1A | 104.6 | -1.0 |
| C8A | O1A | C9A | 105.8 | -0.6 |
| C8A | N1A | C10A | 107.6 | -0.5 |
| C2A | C1A | Sn1A | 114.5 | -4.6 |
| C3A | C2A | C7A | 117.3 | -0.2 |
| C3A | C2A | C1A | 119.2 | 0.0 |
| C7A | C2A | C1A | 123.6 | 0.2 |
| C4A | C3A | C2A | 121.9 | 0.9 |
| C3A | C4A | C5A | 120.2 | -0.3 |
| C6A | C5A | C4A | 119.1 | -0.5 |
| C5A | C6A | C7A | 120.8 | 0.8 |
| C6A | C7A | C2A | 120.7 | -0.8 |
| C6A | C7A | C8A | 117.9 | 0.8 |
| C2A | C7A | C8A | 121.4 | 0.0 |
| N1A | C8A | O1A | 117.3 | 0.3 |
| N1A | C8A | C7A | 126.7 | 0.9 |
| O1A | C8A | C7A | 115.9 | -1.1 |
| O1A | C9A | C10A | 104.1 | 0.4 |
| N1A | C10A | C11A | 111.0 | -2.2 |
| N1A | C10A | C12A | 108.4 | 0.5 |
| C11A | C10A | C12A | 110.9 | 0.0 |
| N1A | C10A | C9A | 102.6 | 0.4 |
| C11A | C10A | C9A | 112.0 | 0.5 |
| C12A | C10A | C9A | 111.6 | 0.7 |
| C18A | C13A | C14A | 117.9 | -0.1 |
| C18A | C13A | Sn1A | 121.7 | -0.1 |
| C14A | C13A | Sn1A | 120.4 | 0.2 |
| C15A | C14A | C13A | 121.3 | 0.1 |
| C16A | C15A | C14A | 119.9 | -0.1 |
| C17A | C16A | C15A | 119.8 | 0.2 |
| C16A | C17A | C18A | 120.0 | 0.9 |
| C13A | C18A | C17A | 121.2 | -1.1 |
| C20A | C19A | C24A | 118.1 | 0.1 |
| C20A | C19A | Sn1A | 120.7 | 1.7 |
| C24A | C19A | Sn1A | 121.2 | -1.8 |
| C21A | C20A | C19A | 121.2 | -0.2 |
| C22A | C21A | C20A | 119.9 | 0.7 |
| C21A | C22A | C23A | 119.7 | -0.2 |
| C22A | C23A | C24A | 120.0 | -0.3 |
| C23A | C24A | C19A | 121.1 | -0.1 |

| | | | | |
|---|---|---|---|---|
| C30A | C25A | C26A | 118.0 | -0.2 |
| C30A | C25A | Sn1A | 126.2 | -3.8 |
| C26A | C25A | Sn1A | 115.8 | 4.0 |
| C27A | C26A | C25A | 121.3 | 0.0 |
| C28A | C27A | C26A | 119.9 | 0.3 |
| C27A | C28A | C29A | 119.7 | -0.1 |
| C28A | C29A | C30A | 120.2 | -0.1 |
| C25A | C30A | C29A | 121.0 | 0.2 |

**Table S7**. B3PW91-GD3BJ calculated bond lengths and differences for Compound **4"**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1B | C19B | 2.1343 | 0.0048 |
| Sn1B | C25B | 2.1357 | 0.0081 |
| Sn1B | C1B | 2.1631 | -0.0099 |
| Sn1B | C13B | 2.1571 | -0.0031 |
| O1B | C8B | 1.3600 | 0.0148 |
| O1B | C9B | 1.4403 | 0.0052 |
| N1B | C8B | 1.2832 | -0.0157 |
| N1B | C10B | 1.4765 | 0.0067 |
| C1B | C2B | 1.4863 | 0.0139 |
| C2B | C3B | 1.4034 | -0.0067 |
| C2B | C7B | 1.4166 | 0.0042 |
| C3B | C4B | 1.3906 | -0.0115 |
| C4B | C5B | 1.3960 | -0.0196 |
| C5B | C6B | 1.3886 | -0.0074 |
| C6B | C7B | 1.4040 | -0.0146 |
| C7B | C8B | 1.4644 | 0.0034 |
| C9B | C10B | 1.5509 | -0.0082 |
| C10B | C12B | 1.5294 | -0.0107 |
| C10B | C11B | 1.5257 | -0.0010 |
| C13B | C14B | 1.4031 | -0.0154 |
| C13B | C18B | 1.4025 | -0.0018 |
| C14B | C15B | 1.3960 | -0.0015 |
| C15B | C16B | 1.3958 | -0.0368 |
| C16B | C17B | 1.3954 | -0.0088 |
| C17B | C18B | 1.3966 | -0.0114 |
| C19B | C20B | 1.4019 | -0.0159 |
| C19B | C24B | 1.4016 | -0.0072 |
| C20B | C21B | 1.3959 | -0.0031 |
| C21B | C22B | 1.3953 | -0.0244 |
| C22B | C23B | 1.3955 | -0.0165 |
| C23B | C24B | 1.3960 | -0.0046 |
| C25B | C30B | 1.4013 | -0.0093 |
| C25B | C26B | 1.4035 | -0.0037 |
| C26B | C27B | 1.3960 | -0.0142 |
| C27B | C28B | 1.3948 | -0.0141 |
| C28B | C29B | 1.3954 | -0.0120 |
| C29B | C30B | 1.3954 | -0.0082 |
| Sn1B | N1B | 2.8175 | 0.4167 |

**Table S8**. B3PW91-GD3BJ calculated bond angles and differences for Compound **4"**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C19B | Sn1B | C25B | 114.0 | -3.6 |
| C19B | Sn1B | C1B | 110.7 | 1.4 |
| C25B | Sn1B | C1B | 121.0 | -4.9 |
| C19B | Sn1B | C13B | 102.9 | 5.6 |
| C25B | Sn1B | C13B | 100.7 | 5.1 |
| C1B | Sn1B | C13B | 104.8 | -1.5 |
| C8B | O1B | C9B | 106.3 | -0.9 |
| C8B | N1B | C10B | 108.0 | -0.4 |
| C2B | C1B | Sn1B | 114.1 | -3.1 |
| C3B | C2B | C7B | 117.3 | -0.4 |
| C3B | C2B | C1B | 119.4 | -0.3 |
| C7B | C2B | C1B | 123.3 | 0.6 |
| C4B | C3B | C2B | 122.0 | 0.1 |
| C5B | C4B | C3B | 120.1 | 0.5 |
| C4B | C5B | C6B | 119.2 | -0.3 |
| C5B | C6B | C7B | 120.9 | 0.7 |
| C6B | C7B | C2B | 120.4 | -0.5 |
| C6B | C7B | C8B | 118.1 | 1.0 |
| C2B | C7B | C8B | 121.4 | -0.4 |
| N1B | C8B | O1B | 117.1 | 0.6 |
| N1B | C8B | C7B | 126.7 | 1.6 |
| O1B | C8B | C7B | 116.0 | -2.1 |
| O1B | C9B | C10B | 104.7 | -0.1 |
| N1B | C10B | C12B | 108.9 | 0.3 |
| N1B | C10B | C11B | 110.6 | -1.4 |
| C12B | C10B | C11B | 110.9 | -0.1 |
| N1B | C10B | C9B | 102.7 | 0.4 |
| C12B | C10B | C9B | 111.6 | 0.9 |
| C11B | C10B | C9B | 111.8 | 0.0 |
| C14B | C13B | C18B | 118.0 | -0.3 |
| C14B | C13B | Sn1B | 120.8 | 0.7 |
| C18B | C13B | Sn1B | 121.2 | -0.3 |
| C13B | C14B | C15B | 121.2 | 0.0 |
| C16B | C15B | C14B | 120.0 | 0.0 |
| C15B | C16B | C17B | 119.7 | 0.8 |
| C18B | C17B | C16B | 120.0 | -0.4 |
| C17B | C18B | C13B | 121.2 | -0.1 |
| C20B | C19B | C24B | 118.1 | 0.0 |
| C20B | C19B | Sn1B | 120.3 | 1.5 |
| C24B | C19B | Sn1B | 121.6 | -1.5 |
| C19B | C20B | C21B | 121.2 | 0.2 |
| C22B | C21B | C20B | 120.0 | -0.1 |
| C21B | C22B | C23B | 119.7 | 0.2 |
| C22B | C23B | C24B | 120.0 | 0.4 |
| C23B | C24B | C19B | 121.1 | -0.7 |

| | | | | |
|---|---|---|---|---|
| C30B | C25B | C26B | 118.1 | -0.6 |
| C30B | C25B | Sn1B | 125.5 | -3.3 |
| C26B | C25B | Sn1B | 116.4 | 3.9 |
| C27B | C26B | C25B | 121.2 | 0.2 |
| C28B | C27B | C26B | 119.9 | 0.1 |
| C27B | C28B | C29B | 119.6 | 0.2 |
| C28B | C29B | C30B | 120.2 | -0.2 |
| C29B | C30B | C25B | 121.0 | 0.3 |

**Table S9**. PBE0-GD3BJ calculated bond lengths and differences for Compound **4"**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1B | C19B | 2.1391 | -0.0001 |
| Sn1B | C25B | 2.1409 | 0.0030 |
| Sn1B | C1B | 2.1656 | -0.0123 |
| Sn1B | C13B | 2.1614 | -0.0074 |
| O1B | C8B | 1.3563 | 0.0185 |
| O1B | C9B | 1.4351 | 0.0104 |
| N1B | C8B | 1.2813 | -0.0138 |
| N1B | C10B | 1.4735 | 0.0097 |
| C1B | C2B | 1.4857 | 0.0145 |
| C2B | C3B | 1.4024 | -0.0058 |
| C2B | C7B | 1.4147 | 0.0060 |
| C3B | C4B | 1.3894 | -0.0103 |
| C4B | C5B | 1.3946 | -0.0182 |
| C5B | C6B | 1.3875 | -0.0063 |
| C6B | C7B | 1.4026 | -0.0131 |
| C7B | C8B | 1.4646 | 0.0032 |
| C9B | C10B | 1.5484 | -0.0058 |
| C10B | C12B | 1.5276 | -0.0089 |
| C10B | C11B | 1.5242 | 0.0005 |
| C13B | C14B | 1.4022 | -0.0145 |
| C13B | C18B | 1.4015 | -0.0007 |
| C14B | C15B | 1.3948 | -0.0003 |
| C15B | C16B | 1.3944 | -0.0354 |
| C16B | C17B | 1.3938 | -0.0072 |
| C17B | C18B | 1.3955 | -0.0104 |
| C19B | C20B | 1.4010 | -0.0150 |
| C19B | C24B | 1.4008 | -0.0063 |
| C20B | C21B | 1.3949 | -0.0021 |
| C21B | C22B | 1.3939 | -0.0230 |
| C22B | C23B | 1.3941 | -0.0151 |
| C23B | C24B | 1.3950 | -0.0036 |
| C25B | C30B | 1.4004 | -0.0084 |
| C25B | C26B | 1.4026 | -0.0028 |
| C26B | C27B | 1.3950 | -0.0131 |
| C27B | C28B | 1.3933 | -0.0126 |
| C28B | C29B | 1.3940 | -0.0105 |
| C29B | C30B | 1.3944 | -0.0073 |
| Sn1B | N1B | 2.8619 | 0.3723 |

**Table S10.** PBE0-GD3BJ calculated bond angles and differences for Compound **4"**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C19B | Sn1B | C25B | 113.7 | -3.3 |
| C19B | Sn1B | C1B | 110.7 | 1.4 |
| C25B | Sn1B | C1B | 121.2 | -5.1 |
| C19B | Sn1B | C13B | 103.1 | 5.4 |
| C25B | Sn1B | C13B | 101.0 | 4.8 |
| C1B | Sn1B | C13B | 104.4 | -1.1 |
| C8B | O1B | C9B | 106.3 | -0.9 |
| C8B | N1B | C10B | 107.9 | -0.2 |
| C2B | C1B | Sn1B | 114.8 | -3.8 |
| C3B | C2B | C7B | 117.3 | -0.3 |
| C3B | C2B | C1B | 119.4 | -0.3 |
| C7B | C2B | C1B | 123.3 | 0.6 |
| C4B | C3B | C2B | 122.0 | 0.1 |
| C5B | C4B | C3B | 120.2 | 0.5 |
| C4B | C5B | C6B | 119.1 | -0.3 |
| C5B | C6B | C7B | 121.0 | 0.7 |
| C6B | C7B | C2B | 120.4 | -0.6 |
| C6B | C7B | C8B | 118.0 | 1.1 |
| C2B | C7B | C8B | 121.5 | -0.4 |
| N1B | C8B | O1B | 117.3 | 0.4 |
| N1B | C8B | C7B | 126.7 | 1.6 |
| O1B | C8B | C7B | 115.8 | -2.0 |
| O1B | C9B | C10B | 104.8 | -0.1 |
| N1B | C10B | C12B | 109.0 | 0.2 |
| N1B | C10B | C11B | 110.6 | -1.4 |
| C12B | C10B | C11B | 110.8 | -0.1 |
| N1B | C10B | C9B | 102.7 | 0.3 |
| C12B | C10B | C9B | 111.6 | 0.9 |
| C11B | C10B | C9B | 111.8 | 0.1 |
| C14B | C13B | C18B | 117.9 | -0.3 |
| C14B | C13B | Sn1B | 120.8 | 0.7 |
| C18B | C13B | Sn1B | 121.3 | -0.4 |
| C13B | C14B | C15B | 121.2 | 0.0 |
| C16B | C15B | C14B | 120.0 | 0.0 |
| C15B | C16B | C17B | 119.7 | 0.8 |
| C18B | C17B | C16B | 120.0 | -0.4 |
| C17B | C18B | C13B | 121.2 | -0.2 |
| C20B | C19B | C24B | 118.0 | 0.0 |
| C20B | C19B | Sn1B | 120.4 | 1.4 |
| C24B | C19B | Sn1B | 121.6 | -1.4 |
| C19B | C20B | C21B | 121.2 | 0.1 |
| C22B | C21B | C20B | 120.0 | -0.1 |
| C21B | C22B | C23B | 119.7 | 0.2 |
| C22B | C23B | C24B | 120.0 | 0.4 |
| C23B | C24B | C19B | 121.1 | -0.7 |

| | | | | |
|---|---|---|---|---|
| C30B | C25B | C26B | 118.0 | -0.6 |
| C30B | C25B | Sn1B | 125.6 | -3.4 |
| C26B | C25B | Sn1B | 116.3 | 4.0 |
| C27B | C26B | C25B | 121.2 | 0.2 |
| C28B | C27B | C26B | 119.9 | 0.1 |
| C27B | C28B | C29B | 119.6 | 0.2 |
| C28B | C29B | C30B | 120.2 | -0.2 |
| C29B | C30B | C25B | 121.0 | 0.3 |

**Table S11**. M05-2X-GD3 calculated bond lengths and differences for Compound **4"**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1B | C19B | 2.1306 | 0.008 |
| Sn1B | C25B | 2.1335 | 0.010 |
| Sn1B | C1B | 2.1576 | -0.004 |
| Sn1B | C13B | 2.1506 | 0.003 |
| O1B | C8B | 1.3614 | 0.013 |
| O1B | C9B | 1.4416 | 0.004 |
| N1B | C8B | 1.2764 | -0.009 |
| N1B | C10B | 1.4770 | 0.006 |
| C1B | C2B | 1.4918 | 0.008 |
| C2B | C3B | 1.4022 | -0.006 |
| C2B | C7B | 1.4114 | 0.009 |
| C3B | C4B | 1.3893 | -0.010 |
| C4B | C5B | 1.3944 | -0.018 |
| C5B | C6B | 1.3877 | -0.006 |
| C6B | C7B | 1.4011 | -0.012 |
| C7B | C8B | 1.4701 | -0.002 |
| C9B | C10B | 1.5444 | -0.002 |
| C10B | C12B | 1.5296 | -0.011 |
| C10B | C11B | 1.5243 | 0.000 |
| C13B | C14B | 1.4023 | -0.015 |
| C13B | C18B | 1.4006 | 0.000 |
| C14B | C15B | 1.3943 | 0.000 |
| C15B | C16B | 1.3944 | -0.035 |
| C16B | C17B | 1.3931 | -0.006 |
| C17B | C18B | 1.3958 | -0.011 |
| C19B | C20B | 1.4007 | -0.015 |
| C19B | C24B | 1.4004 | -0.006 |
| C20B | C21B | 1.3948 | -0.002 |
| C21B | C22B | 1.3940 | -0.023 |
| C22B | C23B | 1.3939 | -0.015 |
| C23B | C24B | 1.3953 | -0.004 |
| C25B | C30B | 1.4002 | -0.008 |
| C25B | C26B | 1.4027 | -0.003 |
| C26B | C27B | 1.3948 | -0.013 |
| C27B | C28B | 1.3929 | -0.012 |
| C28B | C29B | 1.3935 | -0.010 |
| C29B | C30B | 1.3943 | -0.007 |
| Sn1B | N1B | 2.9590 | 0.275 |

**Table S12.** M05-2X-GD3 calculated bond angles and differences for Compound **4"**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C19B | Sn1B | C25B | 112.5 | -2.0 |
| C19B | Sn1B | C1B | 111.3 | 0.8 |
| C25B | Sn1B | C1B | 120.5 | -4.4 |
| C19B | Sn1B | C13B | 104.1 | 4.3 |
| C25B | Sn1B | C13B | 101.7 | 4.1 |
| C1B | Sn1B | C13B | 104.6 | -1.3 |
| C8B | O1B | C9B | 105.8 | -0.4 |
| C8B | N1B | C10B | 107.6 | 0.1 |
| C2B | C1B | Sn1B | 114.5 | -3.5 |
| C3B | C2B | C7B | 117.3 | -0.3 |
| C3B | C2B | C1B | 119.2 | -0.1 |
| C7B | C2B | C1B | 123.6 | 0.3 |
| C4B | C3B | C2B | 121.9 | 0.2 |
| C5B | C4B | C3B | 120.2 | 0.4 |
| C4B | C5B | C6B | 119.1 | -0.3 |
| C5B | C6B | C7B | 120.8 | 0.8 |
| C6B | C7B | C2B | 120.7 | -0.8 |
| C6B | C7B | C8B | 117.9 | 1.2 |
| C2B | C7B | C8B | 121.4 | -0.3 |
| N1B | C8B | O1B | 117.3 | 0.5 |
| N1B | C8B | C7B | 126.7 | 1.6 |
| O1B | C8B | C7B | 115.9 | -2.0 |
| O1B | C9B | C10B | 104.1 | 0.5 |
| N1B | C10B | C12B | 108.4 | 0.8 |
| N1B | C10B | C11B | 111.0 | -1.8 |
| C12B | C10B | C11B | 110.9 | -0.2 |
| N1B | C10B | C9B | 102.6 | 0.5 |
| C12B | C10B | C9B | 111.6 | 0.9 |
| C11B | C10B | C9B | 112.0 | -0.2 |
| C14B | C13B | C18B | 117.9 | -0.3 |
| C14B | C13B | Sn1B | 120.4 | 1.1 |
| C18B | C13B | Sn1B | 121.7 | -0.8 |
| C13B | C14B | C15B | 121.3 | -0.1 |
| C16B | C15B | C14B | 119.9 | 0.1 |
| C15B | C16B | C17B | 119.8 | 0.7 |
| C18B | C17B | C16B | 120.0 | -0.4 |
| C17B | C18B | C13B | 121.2 | -0.1 |
| C20B | C19B | C24B | 118.1 | -0.1 |
| C20B | C19B | Sn1B | 120.7 | 1.1 |
| C24B | C19B | Sn1B | 121.2 | -1.1 |
| C19B | C20B | C21B | 121.2 | 0.2 |
| C22B | C21B | C20B | 119.9 | -0.1 |
| C21B | C22B | C23B | 119.7 | 0.1 |
| C22B | C23B | C24B | 120.0 | 0.4 |
| C23B | C24B | C19B | 121.1 | -0.6 |

| | | | | |
|---|---|---|---|---|
| C30B | C25B | C26B | 118.0 | -0.5 |
| C30B | C25B | Sn1B | 126.2 | -4.0 |
| C26B | C25B | Sn1B | 115.8 | 4.5 |
| C27B | C26B | C25B | 121.3 | 0.2 |
| C28B | C27B | C26B | 119.9 | 0.1 |
| C27B | C28B | C29B | 119.7 | 0.1 |
| C28B | C29B | C30B | 120.2 | -0.2 |
| C29B | C30B | C25B | 121.0 | 0.3 |

**Table S13**. B3PW91-GD3BJ calculated bond lengths and differences for Compound **7**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1 | C18 | 2.1308 | 0.0069 |
| Sn1 | C24 | 2.1331 | 0.0094 |
| Sn1 | C11 | 2.1506 | 0.0096 |
| Sn1 | C12 | 2.1583 | 0.0170 |
| O1 | C1 | 1.3533 | 0.0080 |
| O1 | C2 | 1.4461 | 0.0085 |
| N1 | C1 | 1.2796 | -0.0117 |
| N1 | C3 | 1.4730 | 0.0118 |
| C1 | C6 | 1.4642 | 0.0054 |
| C2 | C3 | 1.5540 | -0.0050 |
| C3 | C4 | 1.5253 | -0.0057 |
| C3 | C5 | 1.5300 | -0.0081 |
| C6 | C7 | 1.3988 | -0.0060 |
| C6 | C11 | 1.4088 | -0.0029 |
| C7 | C8 | 1.3933 | -0.0066 |
| C8 | C9 | 1.3948 | -0.0113 |
| C9 | C10 | 1.3982 | -0.0050 |
| C10 | C11 | 1.3969 | -0.0062 |
| C12 | C17 | 1.4032 | -0.0047 |
| C12 | C13 | 1.4028 | -0.0023 |
| C13 | C14 | 1.3964 | -0.0052 |
| C14 | C15 | 1.3955 | -0.0172 |
| C15 | C16 | 1.3958 | -0.0151 |
| C16 | C17 | 1.3963 | -0.0076 |
| C18 | C19 | 1.4006 | -0.0066 |
| C18 | C23 | 1.4024 | -0.0086 |
| C19 | C20 | 1.3953 | -0.0039 |
| C20 | C21 | 1.3959 | -0.0219 |
| C21 | C22 | 1.3951 | -0.0178 |
| C22 | C23 | 1.3963 | -0.0070 |
| C24 | C25 | 1.4018 | -0.0140 |
| C24 | C29 | 1.4003 | -0.0103 |
| C25 | C26 | 1.3957 | -0.0067 |
| C26 | C27 | 1.3960 | -0.0221 |
| C27 | C28 | 1.3953 | -0.0250 |
| C28 | C29 | 1.3962 | -0.0040 |
| Sn1 | N1 | 2.6873 | 0.0745 |

**Table S14.** B3PW91-GD3BJ calculated bond angles and differences for Compound **7**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C18 | Sn1 | C24 | 118.2 | -3.1 |
| C18 | Sn1 | C11 | 118.4 | -1.3 |
| C24 | Sn1 | C11 | 110.6 | 4.3 |
| C18 | Sn1 | C12 | 101.4 | 0.6 |
| C24 | Sn1 | C12 | 103.0 | -1.0 |
| C11 | Sn1 | C12 | 101.9 | 0.5 |
| C1 | O1 | C2 | 105.7 | -0.3 |
| C1 | N1 | C3 | 108.3 | -0.2 |
| N1 | C1 | O1 | 117.6 | 0.8 |
| N1 | C1 | C6 | 123.6 | 0.4 |
| O1 | C1 | C6 | 118.8 | -1.2 |
| O1 | C2 | C3 | 104.8 | 0.4 |
| N1 | C3 | C4 | 110.6 | -1.0 |
| N1 | C3 | C5 | 109.0 | -0.2 |
| C4 | C3 | C5 | 110.7 | 0.2 |
| N1 | C3 | C2 | 102.2 | 0.5 |
| C4 | C3 | C2 | 112.3 | 0.2 |
| C5 | C3 | C2 | 111.7 | 0.3 |
| C7 | C6 | C11 | 121.4 | -0.4 |
| C7 | C6 | C1 | 120.9 | -0.5 |
| C11 | C6 | C1 | 117.6 | 0.9 |
| C8 | C7 | C6 | 119.5 | 0.5 |
| C9 | C8 | C7 | 119.9 | -0.1 |
| C8 | C9 | C10 | 120.2 | -0.2 |
| C11 | C10 | C9 | 121.0 | 0.4 |
| C10 | C11 | C6 | 117.9 | -0.3 |
| C10 | C11 | Sn1 | 120.4 | -0.2 |
| C6 | C11 | Sn1 | 121.6 | 0.6 |
| C17 | C12 | C13 | 117.9 | -0.8 |
| C17 | C12 | Sn1 | 121.4 | -0.2 |
| C13 | C12 | Sn1 | 120.6 | 1.1 |
| C14 | C13 | C12 | 121.2 | 0.0 |
| C15 | C14 | C13 | 119.9 | 0.3 |
| C14 | C15 | C16 | 119.7 | 0.1 |
| C15 | C16 | C17 | 119.9 | 0.0 |
| C16 | C17 | C12 | 121.2 | 0.4 |
| C19 | C18 | C23 | 118.3 | -0.6 |
| C19 | C18 | Sn1 | 122.5 | 0.5 |
| C23 | C18 | Sn1 | 119.1 | 0.1 |
| C20 | C19 | C18 | 121.0 | -0.2 |
| C21 | C20 | C19 | 120.0 | 0.4 |
| C20 | C21 | C22 | 119.7 | 0.1 |
| C21 | C22 | C23 | 119.9 | 0.0 |
| C22 | C23 | C18 | 121.0 | 0.3 |
| C25 | C24 | C29 | 118.3 | -0.7 |

| | | | | |
|---|---|---|---|---|
| C25 | C24 | Sn1 | 120.1 | 1.1 |
| C29 | C24 | Sn1 | 121.6 | -0.5 |
| C24 | C25 | C26 | 121.0 | 0.1 |
| C27 | C26 | C25 | 120.0 | 0.4 |
| C28 | C27 | C26 | 119.7 | -0.1 |
| C27 | C28 | C29 | 120.0 | 0.2 |
| C24 | C29 | C28 | 121.0 | 0.1 |

**Table S15**. PBE0-GD3BJ calculated bond lengths and differences for Compound **7**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1 | C18 | 2.1362 | 0.0015 |
| Sn1 | C24 | 2.1381 | 0.0044 |
| Sn1 | C11 | 2.1550 | 0.0052 |
| Sn1 | C12 | 2.1641 | 0.0112 |
| O1 | C1 | 1.3498 | 0.0115 |
| O1 | C2 | 1.4403 | 0.0143 |
| N1 | C1 | 1.2780 | -0.0101 |
| N1 | C3 | 1.4712 | 0.0137 |
| C1 | C6 | 1.4639 | 0.0057 |
| C2 | C3 | 1.5505 | -0.0016 |
| C3 | C4 | 1.5234 | -0.0038 |
| C3 | C5 | 1.5282 | -0.0063 |
| C6 | C7 | 1.3975 | -0.0047 |
| C6 | C11 | 1.4069 | -0.0010 |
| C7 | C8 | 1.3919 | -0.0052 |
| C8 | C9 | 1.3933 | -0.0097 |
| C9 | C10 | 1.3969 | -0.0038 |
| C10 | C11 | 1.3961 | -0.0054 |
| C12 | C17 | 1.4023 | -0.0038 |
| C12 | C13 | 1.4018 | -0.0013 |
| C13 | C14 | 1.3954 | -0.0042 |
| C14 | C15 | 1.3940 | -0.0157 |
| C15 | C16 | 1.3943 | -0.0136 |
| C16 | C17 | 1.3951 | -0.0065 |
| C18 | C19 | 1.3996 | -0.0056 |
| C18 | C23 | 1.4014 | -0.0076 |
| C19 | C20 | 1.3943 | -0.0029 |
| C20 | C21 | 1.3944 | -0.0204 |
| C21 | C22 | 1.3936 | -0.0164 |
| C22 | C23 | 1.3952 | -0.0059 |
| C24 | C25 | 1.4008 | -0.0130 |
| C24 | C29 | 1.3997 | -0.0096 |
| C25 | C26 | 1.3948 | -0.0059 |
| C26 | C27 | 1.3945 | -0.0206 |
| C27 | C28 | 1.3939 | -0.0236 |
| C28 | C29 | 1.3951 | -0.0029 |
| Sn1 | N1 | 2.7045 | 0.0574 |

**Table S16.** PBE0-GD3BJ calculated bond angles and differences for Compound **7**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C18 | Sn1 | C24 | 117.8 | -2.7 |
| C18 | Sn1 | C11 | 118.1 | -1.0 |
| C24 | Sn1 | C11 | 111.5 | 3.4 |
| C18 | Sn1 | C12 | 101.4 | 0.7 |
| C24 | Sn1 | C12 | 102.8 | -0.8 |
| C11 | Sn1 | C12 | 101.8 | 0.6 |
| C1 | O1 | C2 | 105.7 | -0.2 |
| C1 | N1 | C3 | 108.0 | 0.1 |
| N1 | C1 | O1 | 117.8 | 0.6 |
| N1 | C1 | C6 | 123.8 | 0.2 |
| O1 | C1 | C6 | 118.4 | -0.9 |
| O1 | C2 | C3 | 104.8 | 0.4 |
| N1 | C3 | C4 | 110.8 | -1.2 |
| N1 | C3 | C5 | 109.1 | -0.4 |
| C4 | C3 | C5 | 110.6 | 0.3 |
| N1 | C3 | C2 | 102.2 | 0.5 |
| C4 | C3 | C2 | 112.2 | 0.3 |
| C5 | C3 | C2 | 111.6 | 0.4 |
| C7 | C6 | C11 | 121.5 | -0.5 |
| C7 | C6 | C1 | 120.7 | -0.3 |
| C11 | C6 | C1 | 117.8 | 0.7 |
| C8 | C7 | C6 | 119.5 | 0.5 |
| C9 | C8 | C7 | 119.8 | -0.1 |
| C8 | C9 | C10 | 120.2 | -0.2 |
| C11 | C10 | C9 | 121.0 | 0.4 |
| C10 | C11 | C6 | 117.8 | -0.2 |
| C10 | C11 | Sn1 | 120.2 | -0.1 |
| C6 | C11 | Sn1 | 121.8 | 0.3 |
| C17 | C12 | C13 | 117.8 | -0.7 |
| C17 | C12 | Sn1 | 121.4 | -0.2 |
| C13 | C12 | Sn1 | 120.7 | 1.0 |
| C14 | C13 | C12 | 121.3 | 0.0 |
| C15 | C14 | C13 | 120.0 | 0.3 |
| C14 | C15 | C16 | 119.7 | 0.1 |
| C15 | C16 | C17 | 119.9 | 0.0 |
| C16 | C17 | C12 | 121.3 | 0.4 |
| C19 | C18 | C23 | 118.2 | -0.5 |
| C19 | C18 | Sn1 | 122.7 | 0.3 |
| C23 | C18 | Sn1 | 119.0 | 0.2 |
| C20 | C19 | C18 | 121.0 | -0.3 |
| C21 | C20 | C19 | 120.0 | 0.4 |
| C20 | C21 | C22 | 119.7 | 0.2 |
| C21 | C22 | C23 | 119.9 | 0.0 |
| C22 | C23 | C18 | 121.0 | 0.2 |
| C25 | C24 | C29 | 118.2 | -0.6 |

| | | | | |
|---|---|---|---|---|
| C25 | C24 | Sn1 | 120.4 | 0.9 |
| C29 | C24 | Sn1 | 121.4 | -0.3 |
| C24 | C25 | C26 | 121.1 | 0.0 |
| C27 | C26 | C25 | 120.0 | 0.4 |
| C28 | C27 | C26 | 119.7 | -0.1 |
| C27 | C28 | C29 | 120.0 | 0.2 |
| C24 | C29 | C28 | 121.0 | 0.1 |

**Table S17**. M05-2X-GD3 calculated bond lengths and differences for Compound **7**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1 | C18 | 2.1303 | 0.0075 |
| Sn1 | C24 | 2.1318 | 0.0107 |
| Sn1 | C11 | 2.1505 | 0.0097 |
| Sn1 | C12 | 2.1578 | 0.0174 |
| O1 | C1 | 1.3535 | 0.0078 |
| O1 | C2 | 1.4469 | 0.0078 |
| N1 | C1 | 1.2737 | -0.0058 |
| N1 | C3 | 1.4753 | 0.0096 |
| C1 | C6 | 1.4695 | 0.0001 |
| C2 | C3 | 1.5471 | 0.0019 |
| C3 | C4 | 1.5242 | -0.0046 |
| C3 | C5 | 1.5300 | -0.0082 |
| C6 | C7 | 1.3956 | -0.0027 |
| C6 | C11 | 1.4050 | 0.0008 |
| C7 | C8 | 1.3922 | -0.0055 |
| C8 | C9 | 1.3925 | -0.0090 |
| C9 | C10 | 1.3972 | -0.0040 |
| C10 | C11 | 1.3965 | -0.0058 |
| C12 | C17 | 1.4023 | -0.0037 |
| C12 | C13 | 1.4014 | -0.0008 |
| C13 | C14 | 1.3956 | -0.0044 |
| C14 | C15 | 1.3933 | -0.0150 |
| C15 | C16 | 1.3941 | -0.0134 |
| C16 | C17 | 1.3949 | -0.0062 |
| C18 | C19 | 1.3995 | -0.0055 |
| C18 | C23 | 1.4012 | -0.0074 |
| C19 | C20 | 1.3943 | -0.0030 |
| C20 | C21 | 1.3940 | -0.0200 |
| C21 | C22 | 1.3931 | -0.0159 |
| C22 | C23 | 1.3952 | -0.0059 |
| C24 | C25 | 1.4007 | -0.0129 |
| C24 | C29 | 1.3993 | -0.0092 |
| C25 | C26 | 1.3948 | -0.0059 |
| C26 | C27 | 1.3943 | -0.0205 |
| C27 | C28 | 1.3935 | -0.0232 |
| C28 | C29 | 1.3953 | -0.0031 |
| Sn1 | N1 | 2.7273 | 0.0346 |

**Table S18.** M05-2X-GD3 calculated bond angles and differences for Compound **7**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C18 | Sn1 | C24 | 117.3 | -2.2 |
| C18 | Sn1 | C11 | 117.9 | -0.8 |
| C24 | Sn1 | C11 | 111.9 | 3.0 |
| C18 | Sn1 | C12 | 101.4 | 0.6 |
| C24 | Sn1 | C12 | 102.9 | -0.9 |
| C11 | Sn1 | C12 | 102.0 | 0.4 |
| C1 | O1 | C2 | 105.3 | 0.1 |
| C1 | N1 | C3 | 107.8 | 0.3 |
| N1 | C1 | O1 | 117.7 | 0.7 |
| N1 | C1 | C6 | 124.0 | 0.0 |
| O1 | C1 | C6 | 118.3 | -0.7 |
| O1 | C2 | C3 | 104.2 | 0.9 |
| N1 | C3 | C4 | 110.8 | -1.2 |
| N1 | C3 | C5 | 108.9 | -0.2 |
| C4 | C3 | C5 | 110.8 | 0.1 |
| N1 | C3 | C2 | 102.2 | 0.6 |
| C4 | C3 | C2 | 112.4 | 0.1 |
| C5 | C3 | C2 | 111.4 | 0.6 |
| C7 | C6 | C11 | 121.9 | -0.9 |
| C7 | C6 | C1 | 120.3 | 0.1 |
| C11 | C6 | C1 | 117.8 | 0.7 |
| C8 | C7 | C6 | 119.3 | 0.7 |
| C9 | C8 | C7 | 119.8 | 0.0 |
| C8 | C9 | C10 | 120.3 | -0.3 |
| C11 | C10 | C9 | 121.1 | 0.4 |
| C10 | C11 | C6 | 117.6 | 0.1 |
| C10 | C11 | Sn1 | 120.1 | 0.0 |
| C6 | C11 | Sn1 | 122.2 | -0.1 |
| C17 | C12 | C13 | 117.8 | -0.7 |
| C17 | C12 | Sn1 | 121.4 | -0.2 |
| C13 | C12 | Sn1 | 120.8 | 0.9 |
| C14 | C13 | C12 | 121.3 | -0.1 |
| C15 | C14 | C13 | 120.0 | 0.3 |
| C14 | C15 | C16 | 119.7 | 0.1 |
| C15 | C16 | C17 | 119.9 | 0.0 |
| C16 | C17 | C12 | 121.3 | 0.3 |
| C19 | C18 | C23 | 118.2 | -0.4 |
| C19 | C18 | Sn1 | 122.9 | 0.1 |
| C23 | C18 | Sn1 | 118.9 | 0.3 |
| C20 | C19 | C18 | 121.0 | -0.3 |
| C21 | C20 | C19 | 120.0 | 0.4 |
| C20 | C21 | C22 | 119.7 | 0.1 |
| C21 | C22 | C23 | 119.9 | 0.0 |
| C22 | C23 | C18 | 121.1 | 0.2 |
| C25 | C24 | C29 | 118.2 | -0.6 |

| | | | | |
|---|---|---|---|---|
| C25 | C24 | Sn1 | 120.6 | 0.6 |
| C29 | C24 | Sn1 | 121.1 | 0.0 |
| C24 | C25 | C26 | 121.1 | 0.0 |
| C27 | C26 | C25 | 119.9 | 0.4 |
| C28 | C27 | C26 | 119.7 | -0.2 |
| C27 | C28 | C29 | 120.0 | 0.2 |
| C24 | C29 | C28 | 121.1 | 0.1 |

**Table S19**. B3PW91-GD3BJ calculated bond lengths and differences for Compound **9'**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1A | C18A | 2.1244 | 0.0006 |
| Sn1A | C12A | 2.1210 | 0.0112 |
| Sn1A | C11A | 2.1483 | -0.0083 |
| Sn1A | N1A | 2.4254 | 0.0404 |
| Sn1A | Cl1A | 2.4335 | 0.0498 |
| O1A | C1A | 1.3438 | -0.0009 |
| O1A | C2A | 1.4515 | 0.0104 |
| N1A | C1A | 1.2858 | -0.0040 |
| N1A | C3A | 1.4763 | 0.0164 |
| C1A | C6A | 1.4591 | 0.0018 |
| C2A | C3A | 1.5474 | -0.0034 |
| C3A | C5A | 1.5219 | -0.0028 |
| C3A | C4A | 1.5315 | -0.0032 |
| C6A | C7A | 1.3976 | -0.0037 |
| C6A | C11A | 1.4090 | -0.0057 |
| C7A | C8A | 1.3933 | -0.0059 |
| C8A | C9A | 1.3957 | -0.0141 |
| C9A | C10A | 1.3990 | -0.0055 |
| C10A | C11A | 1.3936 | -0.0034 |
| C12A | C13A | 1.4010 | -0.0104 |
| C12A | C17A | 1.4000 | 0.0029 |
| C13A | C14A | 1.3962 | -0.0074 |
| C14A | C15A | 1.3953 | -0.0115 |
| C15A | C16A | 1.3959 | -0.0101 |
| C16A | C17A | 1.3953 | -0.0060 |
| C18A | C19A | 1.4005 | -0.0105 |
| C18A | C23A | 1.4011 | -0.0101 |
| C19A | C20A | 1.3951 | -0.0045 |
| C20A | C21A | 1.3956 | -0.0142 |
| C21A | C22A | 1.3951 | -0.0147 |
| C22A | C23A | 1.3960 | -0.0003 |
| Sn1A | N1A | 2.4254 | 0.0404 |

**Table S20.** B3PW91-GD3BJ calculated bond angles and differences for Compound **9'**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C18A | Sn1A | C12A | 115.3 | 2.6 |
| C18A | Sn1A | C11A | 117.5 | 1.9 |
| C12A | Sn1A | C11A | 122.1 | -1.1 |
| C18A | Sn1A | N1A | 88.5 | 1.8 |
| C12A | Sn1A | N1A | 84.9 | 6.8 |
| C11A | Sn1A | N1A | 74.3 | 0.7 |
| C18A | Sn1A | Cl1A | 98.2 | -4.0 |
| C12A | Sn1A | Cl1A | 97.9 | -3.2 |
| C11A | Sn1A | Cl1A | 96.8 | -2.4 |
| N1A | Sn1A | Cl1A | 170.7 | -1.4 |
| C1A | O1A | C2A | 105.4 | 0.3 |
| C1A | N1A | C3A | 108.2 | -0.8 |
| C1A | N1A | Sn1A | 109.6 | -2.6 |
| C3A | N1A | Sn1A | 141.8 | 3.7 |
| N1A | C1A | O1A | 117.0 | 1.0 |
| N1A | C1A | C6A | 122.3 | 1.2 |
| O1A | C1A | C6A | 120.7 | -2.2 |
| O1A | C2A | C3A | 104.4 | -0.1 |
| N1A | C3A | C5A | 111.2 | -0.4 |
| N1A | C3A | C4A | 108.9 | -0.6 |
| C5A | C3A | C4A | 111.2 | 0.7 |
| N1A | C3A | C2A | 100.9 | 1.0 |
| C5A | C3A | C2A | 113.0 | -0.1 |
| C4A | C3A | C2A | 111.2 | -0.7 |
| C7A | C6A | C11A | 121.8 | -0.6 |
| C7A | C6A | C1A | 122.1 | -0.5 |
| C11A | C6A | C1A | 116.1 | 1.0 |
| C8A | C7A | C6A | 119.0 | 0.2 |
| C9A | C8A | C7A | 120.0 | 0.3 |
| C8A | C9A | C10A | 120.6 | -0.1 |
| C11A | C10A | C9A | 120.4 | -0.1 |
| C10A | C11A | C6A | 118.2 | 0.3 |
| C10A | C11A | Sn1A | 124.2 | 0.5 |
| C6A | C11A | Sn1A | 117.6 | -0.8 |
| C13A | C12A | C17A | 118.7 | -0.7 |
| C13A | C12A | Sn1A | 119.4 | 2.6 |
| C17A | C12A | Sn1A | 121.8 | -1.8 |
| C14A | C13A | C12A | 120.8 | 0.4 |
| C15A | C14A | C13A | 120.0 | 0.2 |
| C14A | C15A | C16A | 119.8 | -0.1 |
| C15A | C16A | C17A | 120.1 | 0.1 |
| C16A | C17A | C12A | 120.7 | 0.1 |
| C19A | C18A | C23A | 118.6 | 0.1 |
| C19A | C18A | Sn1A | 121.5 | -1.9 |
| C23A | C18A | Sn1A | 119.9 | 1.7 |

| | | | | |
|---|---|---|---|---|
| C18A | C19A | C20A | 120.9 | -0.1 |
| C21A | C20A | C19A | 119.9 | 0.0 |
| C22A | C21A | C20A | 119.8 | 0.3 |
| C21A | C22A | C23A | 120.1 | -0.1 |
| C18A | C23A | C22A | 120.7 | -0.2 |

**Table S21**. PBE0-GD3BJ calculated bond lengths and differences for Compound **9'**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1A | C18A | 2.1292 | -0.0042 |
| Sn1A | C12A | 2.1256 | 0.0066 |
| Sn1A | C11A | 2.1506 | -0.0106 |
| Sn1A | N1A | 2.4474 | 0.0184 |
| Sn1A | Cl1A | 2.4332 | 0.0500 |
| O1A | C1A | 1.3407 | 0.0022 |
| O1A | C2A | 1.4452 | 0.0167 |
| N1A | C1A | 1.2842 | -0.0024 |
| N1A | C3A | 1.4752 | 0.0175 |
| C1A | C6A | 1.4588 | 0.0020 |
| C2A | C3A | 1.5440 | -0.0001 |
| C3A | C5A | 1.5202 | -0.0011 |
| C3A | C4A | 1.5298 | -0.0016 |
| C6A | C7A | 1.3964 | -0.0025 |
| C6A | C11A | 1.4066 | -0.0033 |
| C7A | C8A | 1.3919 | -0.0045 |
| C8A | C9A | 1.3942 | -0.0126 |
| C9A | C10A | 1.3976 | -0.0042 |
| C10A | C11A | 1.3928 | -0.0026 |
| C12A | C13A | 1.4000 | -0.0094 |
| C12A | C17A | 1.3991 | 0.0039 |
| C13A | C14A | 1.3952 | -0.0064 |
| C14A | C15A | 1.3939 | -0.0101 |
| C15A | C16A | 1.3944 | -0.0087 |
| C16A | C17A | 1.3942 | -0.0049 |
| C18A | C19A | 1.3994 | -0.0094 |
| C18A | C23A | 1.4003 | -0.0092 |
| C19A | C20A | 1.3941 | -0.0035 |
| C20A | C21A | 1.3940 | -0.0127 |
| C21A | C22A | 1.3936 | -0.0133 |
| C22A | C23A | 1.3948 | 0.0009 |
| Sn1A | N1A | 2.4474 | 0.0184 |

**Table S22.** PBE0-GD3BJ calculated bond angles and differences for Compound **9'**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C18A | Sn1A | C12A | 115.4 | 2.5 |
| C18A | Sn1A | C11A | 118.0 | 1.4 |
| C12A | Sn1A | C11A | 121.8 | -0.8 |
| C18A | Sn1A | N1A | 89.0 | 1.3 |
| C12A | Sn1A | N1A | 85.3 | 6.4 |
| C11A | Sn1A | N1A | 74.1 | 0.9 |
| C18A | Sn1A | Cl1A | 98.0 | -3.8 |
| C12A | Sn1A | Cl1A | 97.7 | -3.0 |
| C11A | Sn1A | Cl1A | 96.6 | -2.2 |
| N1A | Sn1A | Cl1A | 170.3 | -0.9 |
| C1A | O1A | C2A | 105.3 | 0.4 |
| C1A | N1A | C3A | 107.9 | -0.5 |
| C1A | N1A | Sn1A | 109.1 | -2.1 |
| C3A | N1A | Sn1A | 142.5 | 3.0 |
| N1A | C1A | O1A | 117.2 | 0.9 |
| N1A | C1A | C6A | 122.6 | 0.9 |
| O1A | C1A | C6A | 120.3 | -1.8 |
| O1A | C2A | C3A | 104.4 | -0.1 |
| N1A | C3A | C5A | 111.5 | -0.7 |
| N1A | C3A | C4A | 109.0 | -0.7 |
| C5A | C3A | C4A | 111.1 | 0.8 |
| N1A | C3A | C2A | 100.9 | 1.0 |
| C5A | C3A | C2A | 112.9 | 0.1 |
| C4A | C3A | C2A | 111.1 | -0.6 |
| C7A | C6A | C11A | 121.8 | -0.6 |
| C7A | C6A | C1A | 121.9 | -0.2 |
| C11A | C6A | C1A | 116.3 | 0.8 |
| C8A | C7A | C6A | 119.0 | 0.1 |
| C9A | C8A | C7A | 119.9 | 0.4 |
| C8A | C9A | C10A | 120.6 | -0.1 |
| C11A | C10A | C9A | 120.4 | -0.1 |
| C10A | C11A | C6A | 118.2 | 0.3 |
| C10A | C11A | Sn1A | 124.0 | 0.7 |
| C6A | C11A | Sn1A | 117.8 | -1.0 |
| C13A | C12A | C17A | 118.7 | -0.6 |
| C13A | C12A | Sn1A | 119.5 | 2.5 |
| C17A | C12A | Sn1A | 121.8 | -1.9 |
| C14A | C13A | C12A | 120.8 | 0.4 |
| C15A | C14A | C13A | 120.0 | 0.2 |
| C14A | C15A | C16A | 119.8 | -0.1 |
| C15A | C16A | C17A | 120.1 | 0.1 |
| C16A | C17A | C12A | 120.7 | 0.0 |
| C19A | C18A | C23A | 118.6 | 0.2 |
| C19A | C18A | Sn1A | 121.8 | -2.3 |
| C23A | C18A | Sn1A | 119.6 | 2.0 |

| | | | | |
|---|---|---|---|---|
| C18A | C19A | C20A | 120.9 | -0.1 |
| C21A | C20A | C19A | 120.0 | 0.0 |
| C22A | C21A | C20A | 119.8 | 0.3 |
| C21A | C22A | C23A | 120.1 | -0.1 |
| C18A | C23A | C22A | 120.7 | -0.2 |

**Table S23**. M05-2X-GD3 calculated bond lengths and differences for Compound **9'**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1A | C18A | 2.1215 | 0.0035 |
| Sn1A | C12A | 2.1175 | 0.0148 |
| Sn1A | C11A | 2.1455 | -0.0055 |
| Sn1A | N1A | 2.4512 | 0.0146 |
| Sn1A | Cl1A | 2.4351 | 0.0481 |
| O1A | C1A | 1.3428 | 0.0000 |
| O1A | C2A | 1.4519 | 0.0100 |
| N1A | C1A | 1.2801 | 0.0017 |
| N1A | C3A | 1.4798 | 0.0130 |
| C1A | C6A | 1.4643 | -0.0035 |
| C2A | C3A | 1.5428 | 0.0011 |
| C3A | C5A | 1.5217 | -0.0027 |
| C3A | C4A | 1.5313 | -0.0030 |
| C6A | C7A | 1.3943 | -0.0005 |
| C6A | C11A | 1.4042 | -0.0010 |
| C7A | C8A | 1.3921 | -0.0047 |
| C8A | C9A | 1.3936 | -0.0121 |
| C9A | C10A | 1.3977 | -0.0043 |
| C10A | C11A | 1.3932 | -0.0030 |
| C12A | C13A | 1.3995 | -0.0089 |
| C12A | C17A | 1.3989 | 0.0040 |
| C13A | C14A | 1.3953 | -0.0065 |
| C14A | C15A | 1.3936 | -0.0098 |
| C15A | C16A | 1.3944 | -0.0087 |
| C16A | C17A | 1.3941 | -0.0048 |
| C18A | C19A | 1.3991 | -0.0091 |
| C18A | C23A | 1.4000 | -0.0089 |
| C19A | C20A | 1.3940 | -0.0034 |
| C20A | C21A | 1.3937 | -0.0123 |
| C21A | C22A | 1.3932 | -0.0129 |
| C22A | C23A | 1.3947 | 0.0011 |
| Sn1A | N1A | 2.4512 | 0.0146 |

**Table S24.** M05-2X-GD3 calculated bond angles and differences for Compound **9'**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C18A | Sn1A | C12A | 115.7 | 2.2 |
| C18A | Sn1A | C11A | 118.4 | 1.0 |
| C12A | Sn1A | C11A | 121.2 | -0.2 |
| C18A | Sn1A | N1A | 89.2 | 1.1 |
| C12A | Sn1A | N1A | 85.2 | 6.5 |
| C11A | Sn1A | N1A | 74.2 | 0.8 |
| C18A | Sn1A | Cl1A | 97.8 | -3.6 |
| C12A | Sn1A | Cl1A | 97.6 | -2.9 |
| C11A | Sn1A | Cl1A | 96.5 | -2.2 |
| N1A | Sn1A | Cl1A | 170.4 | -1.0 |
| C1A | O1A | C2A | 105.2 | 0.5 |
| C1A | N1A | C3A | 107.8 | -0.4 |
| C1A | N1A | Sn1A | 108.9 | -1.8 |
| C3A | N1A | Sn1A | 142.7 | 2.8 |
| N1A | C1A | O1A | 117.1 | 0.9 |
| N1A | C1A | C6A | 122.7 | 0.7 |
| O1A | C1A | C6A | 120.1 | -1.6 |
| O1A | C2A | C3A | 103.9 | 0.4 |
| N1A | C3A | C5A | 111.4 | -0.6 |
| N1A | C3A | C4A | 108.9 | -0.7 |
| C5A | C3A | C4A | 111.2 | 0.7 |
| N1A | C3A | C2A | 100.9 | 1.1 |
| C5A | C3A | C2A | 113.0 | 0.0 |
| C4A | C3A | C2A | 110.9 | -0.4 |
| C7A | C6A | C11A | 122.3 | -1.1 |
| C7A | C6A | C1A | 121.4 | 0.2 |
| C11A | C6A | C1A | 116.3 | 0.8 |
| C8A | C7A | C6A | 118.8 | 0.4 |
| C9A | C8A | C7A | 119.9 | 0.4 |
| C8A | C9A | C10A | 120.7 | -0.2 |
| C11A | C10A | C9A | 120.4 | -0.1 |
| C10A | C11A | C6A | 117.9 | 0.6 |
| C10A | C11A | Sn1A | 124.2 | 0.4 |
| C6A | C11A | Sn1A | 117.8 | -1.0 |
| C13A | C12A | C17A | 118.7 | -0.6 |
| C13A | C12A | Sn1A | 119.7 | 2.3 |
| C17A | C12A | Sn1A | 121.6 | -1.6 |
| C14A | C13A | C12A | 120.8 | 0.3 |
| C15A | C14A | C13A | 119.9 | 0.2 |
| C14A | C15A | C16A | 119.8 | -0.2 |
| C15A | C16A | C17A | 120.0 | 0.1 |
| C16A | C17A | C12A | 120.8 | 0.0 |
| C19A | C18A | C23A | 118.5 | 0.2 |
| C19A | C18A | Sn1A | 121.8 | -2.3 |
| C23A | C18A | Sn1A | 119.7 | 2.0 |

| | | | | |
|---|---|---|---|---|
| C18A | C19A | C20A | 120.9 | -0.2 |
| C21A | C20A | C19A | 119.9 | 0.0 |
| C22A | C21A | C20A | 119.8 | 0.3 |
| C21A | C22A | C23A | 120.0 | -0.1 |
| C18A | C23A | C22A | 120.8 | -0.3 |

**Table S25**. B3PW91-GD3BJ calculated bond lengths and differences for Compound **9"**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1B | C18B | 2.1244 | -0.0011 |
| Sn1B | C12B | 2.1210 | 0.0121 |
| Sn1B | C11B | 2.1483 | -0.0062 |
| Sn1B | N1B | 2.4254 | 0.0247 |
| Sn1B | Cl1B | 2.4335 | 0.0620 |
| O1B | C1B | 1.3438 | -0.0040 |
| O1B | C2B | 1.4515 | 0.0055 |
| N1B | C1B | 1.2858 | -0.0011 |
| N1B | C3B | 1.4763 | 0.0154 |
| C1B | C6B | 1.4591 | 0.0097 |
| C2B | C3B | 1.5474 | -0.0001 |
| C3B | C5B | 1.5219 | -0.0001 |
| C3B | C4B | 1.5315 | -0.0058 |
| C6B | C7B | 1.3976 | -0.0086 |
| C6B | C11B | 1.4090 | -0.0071 |
| C7B | C8B | 1.3933 | -0.0079 |
| C8B | C9B | 1.3957 | -0.0115 |
| C9B | C10B | 1.3990 | -0.0029 |
| C10B | C11B | 1.3936 | -0.0012 |
| C12B | C17B | 1.4000 | -0.0077 |
| C12B | C13B | 1.4010 | -0.0065 |
| C13B | C14B | 1.3962 | -0.0062 |
| C14B | C15B | 1.3953 | -0.0116 |
| C15B | C16B | 1.3959 | -0.0135 |
| C16B | C17B | 1.3953 | -0.0065 |
| C18B | C23B | 1.4011 | -0.0102 |
| C18B | C19B | 1.4005 | -0.0093 |
| C19B | C20B | 1.3951 | -0.0055 |
| C20B | C21B | 1.3956 | -0.0136 |
| C21B | C22B | 1.3951 | -0.0120 |
| C22B | C23B | 1.3960 | -0.0124 |
| Sn1B | N1B | 2.4254 | 0.0247 |

**Table S26.** B3PW91-GD3BJ calculated bond angles and differences for Compound **9"**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C18B | Sn1B | C12B | 115.3 | 6.2 |
| C18B | Sn1B | C11B | 117.5 | 0.7 |
| C12B | Sn1B | C11B | 122.1 | -3.5 |
| C18B | Sn1B | N1B | 88.5 | 0.5 |
| C12B | Sn1B | N1B | 84.9 | 7.0 |
| C11B | Sn1B | N1B | 74.3 | 0.9 |
| C18B | Sn1B | Cl1B | 98.2 | -5.1 |
| C12B | Sn1B | Cl1B | 97.9 | -2.9 |
| C11B | Sn1B | Cl1B | 96.8 | -1.2 |
| N1B | Sn1B | Cl1B | 170.7 | -0.3 |
| C1B | O1B | C2B | 105.4 | 0.4 |
| C1B | N1B | C3B | 108.2 | -0.8 |
| C1B | N1B | Sn1B | 109.6 | -2.6 |
| C3B | N1B | Sn1B | 141.8 | 2.9 |
| N1B | C1B | O1B | 117.0 | 1.2 |
| N1B | C1B | C6B | 122.3 | 0.8 |
| O1B | C1B | C6B | 120.7 | -2.0 |
| O1B | C2B | C3B | 104.4 | 0.2 |
| N1B | C3B | C5B | 111.2 | -0.5 |
| N1B | C3B | C4B | 108.9 | -0.2 |
| C5B | C3B | C4B | 111.2 | 0.2 |
| N1B | C3B | C2B | 100.9 | 1.0 |
| C5B | C3B | C2B | 113.0 | -0.2 |
| C4B | C3B | C2B | 111.2 | -0.2 |
| C7B | C6B | C11B | 121.8 | 0.2 |
| C7B | C6B | C1B | 122.1 | -0.9 |
| C11B | C6B | C1B | 116.1 | 0.7 |
| C8B | C7B | C6B | 119.0 | -0.1 |
| C9B | C8B | C7B | 120.0 | 0.4 |
| C8B | C9B | C10B | 120.6 | -0.1 |
| C11B | C10B | C9B | 120.4 | -0.2 |
| C10B | C11B | C6B | 118.2 | -0.1 |
| C10B | C11B | Sn1B | 124.2 | 1.2 |
| C6B | C11B | Sn1B | 117.6 | -1.0 |
| C17B | C12B | C13B | 118.7 | -0.3 |
| C17B | C12B | Sn1B | 121.8 | -1.1 |
| C13B | C12B | Sn1B | 119.4 | 1.3 |
| C14B | C13B | C12B | 120.8 | 0.0 |
| C15B | C14B | C13B | 120.0 | 0.1 |
| C16B | C15B | C14B | 119.8 | 0.1 |
| C15B | C16B | C17B | 120.1 | 0.0 |
| C16B | C17B | C12B | 120.7 | 0.2 |
| C23B | C18B | C19B | 118.6 | -0.2 |
| C23B | C18B | Sn1B | 119.9 | 2.8 |
| C19B | C18B | Sn1B | 121.5 | -2.6 |

| | | | | |
|---|---|---|---|---|
| C20B | C19B | C18B | 120.9 | 0.0 |
| C21B | C20B | C19B | 119.9 | 0.0 |
| C20B | C21B | C22B | 119.8 | -0.1 |
| C23B | C22B | C21B | 120.1 | 0.3 |
| C22B | C23B | C18B | 120.7 | 0.1 |

**Table S27**. PBE0-GD3BJ calculated bond lengths and differences for Compound **9"**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1B | C18B | 2.1292 | -0.0059 |
| Sn1B | C12B | 2.1256 | 0.0075 |
| Sn1B | C11B | 2.1506 | -0.0085 |
| Sn1B | N1B | 2.4474 | 0.0028 |
| Sn1B | Cl1B | 2.4332 | 0.0623 |
| O1B | C1B | 1.3407 | -0.0009 |
| O1B | C2B | 1.4452 | 0.0118 |
| N1B | C1B | 1.2842 | 0.0006 |
| N1B | C3B | 1.4752 | 0.0165 |
| C1B | C6B | 1.4588 | 0.0099 |
| C2B | C3B | 1.5440 | 0.0032 |
| C3B | C5B | 1.5202 | 0.0016 |
| C3B | C4B | 1.5298 | -0.0041 |
| C6B | C7B | 1.3964 | -0.0074 |
| C6B | C11B | 1.4066 | -0.0047 |
| C7B | C8B | 1.3919 | -0.0065 |
| C8B | C9B | 1.3942 | -0.0101 |
| C9B | C10B | 1.3976 | -0.0016 |
| C10B | C11B | 1.3928 | -0.0005 |
| C12B | C17B | 1.3991 | -0.0068 |
| C12B | C13B | 1.4000 | -0.0054 |
| C13B | C14B | 1.3952 | -0.0052 |
| C14B | C15B | 1.3939 | -0.0101 |
| C15B | C16B | 1.3944 | -0.0121 |
| C16B | C17B | 1.3942 | -0.0054 |
| C18B | C23B | 1.4003 | -0.0093 |
| C18B | C19B | 1.3994 | -0.0082 |
| C19B | C20B | 1.3941 | -0.0045 |
| C20B | C21B | 1.3940 | -0.0121 |
| C21B | C22B | 1.3936 | -0.0106 |
| C22B | C23B | 1.3948 | -0.0112 |
| Sn1B | N1B | 2.4474 | 0.0028 |

**Table S28.** PBE0-GD3BJ calculated bond angles and differences for Compound **9"**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C18B | Sn1B | C12B | 115.4 | 6.1 |
| C18B | Sn1B | C11B | 118.0 | 0.2 |
| C12B | Sn1B | C11B | 121.8 | -3.3 |
| C18B | Sn1B | N1B | 89.0 | 0.0 |
| C12B | Sn1B | N1B | 85.3 | 6.6 |
| C11B | Sn1B | N1B | 74.1 | 1.2 |
| C18B | Sn1B | Cl1B | 98.0 | -4.9 |
| C12B | Sn1B | Cl1B | 97.7 | -2.7 |
| C11B | Sn1B | Cl1B | 96.6 | -1.0 |
| N1B | Sn1B | Cl1B | 170.3 | 0.1 |
| C1B | O1B | C2B | 105.3 | 0.4 |
| C1B | N1B | C3B | 107.9 | -0.4 |
| C1B | N1B | Sn1B | 109.1 | -2.1 |
| C3B | N1B | Sn1B | 142.5 | 2.2 |
| N1B | C1B | O1B | 117.2 | 1.0 |
| N1B | C1B | C6B | 122.6 | 0.5 |
| O1B | C1B | C6B | 120.3 | -1.5 |
| O1B | C2B | C3B | 104.4 | 0.2 |
| N1B | C3B | C5B | 111.5 | -0.8 |
| N1B | C3B | C4B | 109.0 | -0.3 |
| C5B | C3B | C4B | 111.1 | 0.3 |
| N1B | C3B | C2B | 100.9 | 1.0 |
| C5B | C3B | C2B | 112.9 | 0.0 |
| C4B | C3B | C2B | 111.1 | -0.1 |
| C7B | C6B | C11B | 121.8 | 0.1 |
| C7B | C6B | C1B | 121.9 | -0.7 |
| C11B | C6B | C1B | 116.3 | 0.5 |
| C8B | C7B | C6B | 119.0 | -0.1 |
| C9B | C8B | C7B | 119.9 | 0.4 |
| C8B | C9B | C10B | 120.6 | -0.1 |
| C11B | C10B | C9B | 120.4 | -0.2 |
| C10B | C11B | C6B | 118.2 | -0.1 |
| C10B | C11B | Sn1B | 124.0 | 1.4 |
| C6B | C11B | Sn1B | 117.8 | -1.3 |
| C17B | C12B | C13B | 118.7 | -0.3 |
| C17B | C12B | Sn1B | 121.8 | -1.2 |
| C13B | C12B | Sn1B | 119.5 | 1.2 |
| C14B | C13B | C12B | 120.8 | 0.0 |
| C15B | C14B | C13B | 120.0 | 0.0 |
| C16B | C15B | C14B | 119.8 | 0.2 |
| C15B | C16B | C17B | 120.1 | -0.1 |
| C16B | C17B | C12B | 120.7 | 0.1 |
| C23B | C18B | C19B | 118.6 | -0.2 |
| C23B | C18B | Sn1B | 119.6 | 3.0 |
| C19B | C18B | Sn1B | 121.8 | -2.9 |

| | | | | |
|---|---|---|---|---|
| C20B | C19B | C18B | 120.9 | 0.0 |
| C21B | C20B | C19B | 120.0 | 0.0 |
| C20B | C21B | C22B | 119.8 | -0.1 |
| C23B | C22B | C21B | 120.1 | 0.2 |
| C22B | C23B | C18B | 120.7 | 0.1 |

**Table S29**. M05-2X-GD3 calculated bond lengths and differences for Compound **9"**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1B | C18B | 2.1215 | 0.0018 |
| Sn1B | C12B | 2.1175 | 0.0157 |
| Sn1B | C11B | 2.1455 | -0.0034 |
| Sn1B | N1B | 2.4512 | -0.0010 |
| Sn1B | Cl1B | 2.4351 | 0.0604 |
| O1B | C1B | 1.3428 | -0.0031 |
| O1B | C2B | 1.4519 | 0.0051 |
| N1B | C1B | 1.2801 | 0.0046 |
| N1B | C3B | 1.4798 | 0.0119 |
| C1B | C6B | 1.4643 | 0.0044 |
| C2B | C3B | 1.5428 | 0.0044 |
| C3B | C5B | 1.5217 | 0.0001 |
| C3B | C4B | 1.5313 | -0.0056 |
| C6B | C7B | 1.3943 | -0.0053 |
| C6B | C11B | 1.4042 | -0.0024 |
| C7B | C8B | 1.3921 | -0.0067 |
| C8B | C9B | 1.3936 | -0.0095 |
| C9B | C10B | 1.3977 | -0.0017 |
| C10B | C11B | 1.3932 | -0.0009 |
| C12B | C17B | 1.3989 | -0.0066 |
| C12B | C13B | 1.3995 | -0.0050 |
| C13B | C14B | 1.3953 | -0.0053 |
| C14B | C15B | 1.3936 | -0.0099 |
| C15B | C16B | 1.3944 | -0.0120 |
| C16B | C17B | 1.3941 | -0.0053 |
| C18B | C23B | 1.4000 | -0.0090 |
| C18B | C19B | 1.3991 | -0.0079 |
| C19B | C20B | 1.3940 | -0.0044 |
| C20B | C21B | 1.3937 | -0.0117 |
| C21B | C22B | 1.3932 | -0.0102 |
| C22B | C23B | 1.3947 | -0.0111 |
| Sn1B | N1B | 2.4512 | -0.0010 |

**Table S30.** M05-2X-GD3 calculated bond angles and differences for Compound **9"**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C18B | Sn1B | C12B | 115.7 | 5.7 |
| C18B | Sn1B | C11B | 118.4 | -0.2 |
| C12B | Sn1B | C11B | 121.2 | -2.7 |
| C18B | Sn1B | N1B | 89.2 | -0.2 |
| C12B | Sn1B | N1B | 85.2 | 6.7 |
| C11B | Sn1B | N1B | 74.2 | 1.0 |
| C18B | Sn1B | Cl1B | 97.8 | -4.7 |
| C12B | Sn1B | Cl1B | 97.6 | -2.7 |
| C11B | Sn1B | Cl1B | 96.5 | -1.0 |
| N1B | Sn1B | Cl1B | 170.4 | 0.1 |
| C1B | O1B | C2B | 105.2 | 0.5 |
| C1B | N1B | C3B | 107.8 | -0.3 |
| C1B | N1B | Sn1B | 108.9 | -1.8 |
| C3B | N1B | Sn1B | 142.7 | 2.0 |
| N1B | C1B | O1B | 117.1 | 1.0 |
| N1B | C1B | C6B | 122.7 | 0.3 |
| O1B | C1B | C6B | 120.1 | -1.4 |
| O1B | C2B | C3B | 103.9 | 0.7 |
| N1B | C3B | C5B | 111.4 | -0.8 |
| N1B | C3B | C4B | 108.9 | -0.3 |
| C5B | C3B | C4B | 111.2 | 0.2 |
| N1B | C3B | C2B | 100.9 | 1.0 |
| C5B | C3B | C2B | 113.0 | -0.2 |
| C4B | C3B | C2B | 110.9 | 0.1 |
| C7B | C6B | C11B | 122.3 | -0.4 |
| C7B | C6B | C1B | 121.4 | -0.2 |
| C11B | C6B | C1B | 116.3 | 0.6 |
| C8B | C7B | C6B | 118.8 | 0.1 |
| C9B | C8B | C7B | 119.9 | 0.4 |
| C8B | C9B | C10B | 120.7 | -0.2 |
| C11B | C10B | C9B | 120.4 | -0.2 |
| C10B | C11B | C6B | 117.9 | 0.2 |
| C10B | C11B | Sn1B | 124.2 | 1.1 |
| C6B | C11B | Sn1B | 117.8 | -1.3 |
| C17B | C12B | C13B | 118.7 | -0.3 |
| C17B | C12B | Sn1B | 121.6 | -1.0 |
| C13B | C12B | Sn1B | 119.7 | 1.0 |
| C14B | C13B | C12B | 120.8 | -0.1 |
| C15B | C14B | C13B | 119.9 | 0.1 |
| C16B | C15B | C14B | 119.8 | 0.1 |
| C15B | C16B | C17B | 120.0 | 0.0 |
| C16B | C17B | C12B | 120.8 | 0.1 |
| C23B | C18B | C19B | 118.5 | -0.1 |
| C23B | C18B | Sn1B | 119.7 | 3.0 |
| C19B | C18B | Sn1B | 121.8 | -2.9 |

| | | | | |
|---|---|---|---|---|
| C20B | C19B | C18B | 120.9 | -0.1 |
| C21B | C20B | C19B | 119.9 | 0.0 |
| C20B | C21B | C22B | 119.8 | -0.1 |
| C23B | C22B | C21B | 120.0 | 0.3 |
| C22B | C23B | C18B | 120.8 | 5.7 |

**Table S31**. B3PW91-GD3BJ calculated bond lengths and differences for Compound **10**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1 | C12 | 2.1159 | 0.0111 |
| Sn1 | C1 | 2.1458 | -0.0098 |
| Sn1 | N1 | 2.4008 | -0.0176 |
| Sn1 | Br1 | 2.5201 | -0.0259 |
| Sn1 | Br2 | 2.5876 | 0.0302 |
| O1A | C7 | 1.3400 | -0.0009 |
| O1A | C8A | 1.4518 | 0.0237 |
| N1 | C7 | 1.2858 | 0.0004 |
| N1 | C9 | 1.4777 | 0.0161 |
| C1 | C2 | 1.3919 | -0.0084 |
| C1 | C6 | 1.4073 | -0.0085 |
| C2 | C3 | 1.3993 | -0.0066 |
| C3 | C4 | 1.3950 | -0.0111 |
| C4 | C5 | 1.3939 | -0.0080 |
| C5 | C6 | 1.3966 | -0.0059 |
| C6 | C7 | 1.4589 | 0.0016 |
| C8A | C9 | 1.5494 | -0.0053 |
| C9 | C10 | 1.5219 | -0.0092 |
| C9 | C11 | 1.5307 | -0.0105 |
| C12 | C17 | 1.3990 | -0.0133 |
| C12 | C13 | 1.3995 | -0.0115 |
| C13 | C14 | 1.3952 | -0.0034 |
| C14 | C15 | 1.3957 | -0.0113 |
| C15 | C16 | 1.3954 | 0.0111 |
| C16 | C17 | 1.3960 | -0.0098 |

**Table S32.** B3PW91-GD3BJ calculated bond angles and differences for Compound **10**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C12 | Sn1 | C1 | 127.8 | -1.0 |
| C12 | Sn1 | N1 | 85.7 | 4.2 |
| C1 | Sn1 | N1 | 74.8 | 1.2 |
| C12 | Sn1 | Br1 | 111.3 | 0.9 |
| C1 | Sn1 | Br1 | 115.2 | 3.0 |
| N1 | Sn1 | Br1 | 86.4 | 1.5 |
| C12 | Sn1 | Br2 | 99.0 | -0.8 |
| C1 | Sn1 | Br2 | 97.2 | -0.8 |
| N1 | Sn1 | Br2 | 172.1 | -0.7 |
| Br1 | Sn1 | Br2 | 97.8 | -5.8 |
| C7 | O1A | C8A | 105.5 | -0.8 |
| C7 | N1 | C9 | 108.4 | -0.3 |
| C7 | N1 | Sn1 | 109.8 | -1.2 |
| C9 | N1 | Sn1 | 141.6 | 1.5 |
| C2 | C1 | C6 | 118.7 | 0.6 |
| C2 | C1 | Sn1 | 124.4 | 0.5 |
| C6 | C1 | Sn1 | 116.9 | -1.1 |
| C1 | C2 | C3 | 120.1 | -0.4 |
| C4 | C3 | C2 | 120.6 | -0.2 |
| C3 | C4 | C5 | 120.1 | 0.5 |
| C4 | C5 | C6 | 119.0 | -0.2 |
| C5 | C6 | C1 | 121.5 | -0.4 |
| C5 | C6 | C7 | 122.3 | -0.1 |
| C1 | C6 | C7 | 116.2 | 0.5 |
| N1 | C7 | O1A | 117.2 | 0.5 |
| N1 | C7 | C6 | 122.2 | 0.7 |
| O1A | C7 | C6 | 120.6 | -1.4 |
| O1A | C8A | C9 | 104.7 | -0.3 |
| N1 | C9 | C10 | 111.3 | -0.3 |
| N1 | C9 | C11 | 109.1 | 0.2 |
| C10 | C9 | C11 | 111.2 | 0.1 |
| N1 | C9 | C8A | 101.0 | 0.4 |
| C10 | C9 | C8A | 112.4 | -3.1 |
| C11 | C9 | C8A | 111.4 | 2.7 |
| C17 | C12 | C13 | 119.4 | 0.0 |
| C17 | C12 | Sn1 | 119.9 | 1.5 |
| C13 | C12 | Sn1 | 120.7 | -1.5 |
| C12 | C13 | C14 | 120.3 | 0.2 |
| C15 | C14 | C13 | 120.0 | -0.6 |
| C16 | C15 | C14 | 119.9 | 0.6 |
| C15 | C16 | C17 | 120.1 | -0.1 |
| C12 | C17 | C16 | 120.3 | -0.1 |

**Table S33**. PBE0-GD3BJ calculated bond lengths and differences for Compound **10**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1 | C12 | 2.1280 | -0.0010 |
| Sn1 | C1 | 2.1525 | -0.0165 |
| Sn1 | N1 | 2.4475 | -0.0643 |
| Sn1 | Br1 | 2.5244 | -0.0302 |
| Sn1 | Br2 | 2.5917 | 0.0262 |
| O1A | C7 | 1.3377 | 0.0015 |
| O1A | C8A | 1.4441 | 0.0314 |
| N1 | C7 | 1.2838 | 0.0023 |
| N1 | C9 | 1.4778 | 0.0160 |
| C1 | C2 | 1.3920 | -0.0085 |
| C1 | C6 | 1.4049 | -0.0061 |
| C2 | C3 | 1.3982 | -0.0055 |
| C3 | C4 | 1.3935 | -0.0096 |
| C4 | C5 | 1.3925 | -0.0066 |
| C5 | C6 | 1.3961 | -0.0053 |
| C6 | C7 | 1.4599 | 0.0006 |
| C8A | C9 | 1.5476 | -0.0036 |
| C9 | C10 | 1.5223 | -0.0096 |
| C9 | C11 | 1.5300 | -0.0098 |
| C12 | C17 | 1.3988 | -0.0131 |
| C12 | C13 | 1.3995 | -0.0115 |
| C13 | C14 | 1.3947 | -0.0029 |
| C14 | C15 | 1.3942 | -0.0098 |
| C15 | C16 | 1.3939 | -0.0010 |
| C16 | C17 | 1.3954 | -0.0165 |

**Table S34.** PBE0-GD3BJ calculated bond angles and differences for Compound **10**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C12 | Sn1 | C1 | 126.9 | -0.2 |
| C12 | Sn1 | N1 | 87.6 | 2.3 |
| C1 | Sn1 | N1 | 74.3 | 1.7 |
| C12 | Sn1 | Br1 | 111.8 | 0.3 |
| C1 | Sn1 | Br1 | 116.1 | 2.1 |
| N1 | Sn1 | Br1 | 86.3 | 1.6 |
| C12 | Sn1 | Br2 | 98.6 | -0.4 |
| C1 | Sn1 | Br2 | 97.2 | -0.8 |
| N1 | Sn1 | Br2 | 171.5 | -0.1 |
| Br1 | Sn1 | Br2 | 96.8 | -4.8 |
| C7 | O1A | C8A | 105.6 | -0.8 |
| C7 | N1 | C9 | 108.0 | 0.2 |
| C7 | N1 | Sn1 | 108.9 | -0.3 |
| C9 | N1 | Sn1 | 143.0 | 0.2 |
| C2 | C1 | C6 | 118.6 | 0.7 |
| C2 | C1 | Sn1 | 124.0 | 0.8 |
| C6 | C1 | Sn1 | 117.4 | -1.6 |
| C1 | C2 | C3 | 120.2 | -0.4 |
| C4 | C3 | C2 | 120.6 | -0.2 |
| C3 | C4 | C5 | 120.0 | 0.6 |
| C4 | C5 | C6 | 119.1 | -0.3 |
| C5 | C6 | C1 | 121.5 | -0.4 |
| C5 | C6 | C7 | 121.8 | 0.4 |
| C1 | C6 | C7 | 116.6 | 0.0 |
| N1 | C7 | O1A | 117.5 | 0.2 |
| N1 | C7 | C6 | 122.7 | 0.1 |
| O1A | C7 | C6 | 119.8 | -0.6 |
| O1A | C8A | C9 | 104.8 | -0.4 |
| N1 | C9 | C10 | 111.7 | -0.7 |
| N1 | C9 | C11 | 109.1 | 0.1 |
| C10 | C9 | C11 | 111.1 | 0.2 |
| N1 | C9 | C8A | 101.2 | 0.2 |
| C10 | C9 | C8A | 112.0 | -2.6 |
| C11 | C9 | C8A | 111.4 | 2.7 |
| C17 | C12 | C13 | 119.1 | 0.3 |
| C17 | C12 | Sn1 | 120.1 | 1.3 |
| C13 | C12 | Sn1 | 120.7 | -1.6 |
| C12 | C13 | C14 | 120.5 | 0.1 |
| C15 | C14 | C13 | 120.1 | -0.6 |
| C16 | C15 | C14 | 119.8 | 0.6 |
| C15 | C16 | C17 | 120.1 | -0.2 |
| C12 | C17 | C16 | 120.4 | -0.2 |

**Table S35**. M05-2X-GD3 calculated bond lengths and differences for Compound **10**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1 | C12 | 2.1099 | 0.0171 |
| Sn1 | C1 | 2.1407 | -0.0047 |
| Sn1 | N1 | 2.4068 | -0.0236 |
| Sn1 | Br1 | 2.5205 | -0.0263 |
| Sn1 | Br2 | 2.5899 | 0.0279 |
| O1A | C7 | 1.3385 | 0.0006 |
| O1A | C8A | 1.4530 | 0.0225 |
| N1 | C7 | 1.2800 | 0.0061 |
| N1 | C9 | 1.4805 | 0.0132 |
| C1 | C2 | 1.3915 | -0.0080 |
| C1 | C6 | 1.4030 | -0.0042 |
| C2 | C3 | 1.3982 | -0.0056 |
| C3 | C4 | 1.3930 | -0.0091 |
| C4 | C5 | 1.3927 | -0.0069 |
| C5 | C6 | 1.3931 | -0.0024 |
| C6 | C7 | 1.4640 | -0.0035 |
| C8A | C9 | 1.5453 | -0.0012 |
| C9 | C10 | 1.5219 | -0.0092 |
| C9 | C11 | 1.5305 | -0.0103 |
| C12 | C17 | 1.3976 | -0.0119 |
| C12 | C13 | 1.3985 | -0.0106 |
| C13 | C14 | 1.3939 | -0.0021 |
| C14 | C15 | 1.3941 | -0.0098 |
| C15 | C16 | 1.3937 | 0.0111 |
| C16 | C17 | 1.3951 | -0.0098 |

**Table S36.** M05-2X-GD3 calculated bond angles and differences for Compound **10**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C12 | Sn1 | C1 | 126.3 | 0.5 |
| C12 | Sn1 | N1 | 86.3 | 3.5 |
| C1 | Sn1 | N1 | 75.0 | 1.1 |
| C12 | Sn1 | Br1 | 111.8 | 0.3 |
| C1 | Sn1 | Br1 | 116.7 | 1.5 |
| N1 | Sn1 | Br1 | 86.7 | 1.2 |
| C12 | Sn1 | Br2 | 98.9 | -0.7 |
| C1 | Sn1 | Br2 | 97.2 | -0.7 |
| N1 | Sn1 | Br2 | 172.2 | -0.8 |
| Br1 | Sn1 | Br2 | 96.7 | -4.7 |
| C7 | O1A | C8A | 105.4 | -0.6 |
| C7 | N1 | C9 | 108.1 | 0.1 |
| C7 | N1 | Sn1 | 109.4 | -0.8 |
| C9 | N1 | Sn1 | 142.3 | 0.9 |
| C2 | C1 | C6 | 118.3 | 1.0 |
| C2 | C1 | Sn1 | 124.8 | 0.0 |
| C6 | C1 | Sn1 | 116.9 | -1.1 |
| C1 | C2 | C3 | 120.2 | -0.4 |
| C4 | C3 | C2 | 120.7 | -0.3 |
| C3 | C4 | C5 | 120.0 | 0.6 |
| C4 | C5 | C6 | 118.8 | 0.0 |
| C5 | C6 | C1 | 122.1 | -1.0 |
| C5 | C6 | C7 | 121.7 | 0.6 |
| C1 | C6 | C7 | 116.2 | 0.4 |
| N1 | C7 | O1A | 117.3 | 0.4 |
| N1 | C7 | C6 | 122.4 | 0.4 |
| O1A | C7 | C6 | 120.3 | -1.0 |
| O1A | C8A | C9 | 104.2 | 0.2 |
| N1 | C9 | C10 | 111.5 | -0.6 |
| N1 | C9 | C11 | 109.1 | 0.1 |
| C10 | C9 | C11 | 111.2 | 0.1 |
| N1 | C9 | C8A | 100.9 | 0.5 |
| C10 | C9 | C8A | 112.4 | -3.0 |
| C11 | C9 | C8A | 111.2 | 2.9 |
| C17 | C12 | C13 | 119.3 | 0.1 |
| C17 | C12 | Sn1 | 120.3 | 1.1 |
| C13 | C12 | Sn1 | 120.3 | -1.1 |
| C12 | C13 | C14 | 120.4 | 0.1 |
| C15 | C14 | C13 | 120.0 | -0.5 |
| C16 | C15 | C14 | 119.9 | 0.5 |
| C15 | C16 | C17 | 120.1 | -0.1 |
| C12 | C17 | C16 | 120.3 | -0.1 |

**Table S37**. B3PW91-GD3BJ calculated bond lengths and differences for Compound **11**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1 | C1 | 2.1465 | -0.0202 |
| Sn1 | C13 | 2.1164 | 0.0139 |
| Sn1 | N1 | 2.4687 | -0.0440 |
| Sn1 | Br2 | 2.5276 | -0.0109 |
| Sn1 | Br1 | 2.5886 | 0.0508 |
| O1 | C8 | 1.3483 | -0.0023 |
| O1 | C10 | 1.4416 | -0.0059 |
| N1 | C8 | 1.2932 | -0.0033 |
| N1 | C9 | 1.4863 | -0.0032 |
| C1 | C2 | 1.4874 | 0.0059 |
| C2 | C3 | 1.4003 | -0.0110 |
| C2 | C7 | 1.4148 | -0.0118 |
| C3 | C4 | 1.3913 | -0.0058 |
| C4 | C5 | 1.3958 | -0.0257 |
| C5 | C6 | 1.3880 | -0.0087 |
| C6 | C7 | 1.4038 | 0.0038 |
| C7 | C8 | 1.4602 | 0.0052 |
| C9 | C11 | 1.5296 | -0.0107 |
| C9 | C12 | 1.5232 | -0.0039 |
| C9 | C10 | 1.5422 | 0.0003 |
| C13 | C18 | 1.3993 | -0.0113 |
| C13 | C14 | 1.3997 | -0.0055 |
| C14 | C15 | 1.3946 | -0.0077 |
| C15 | C16 | 1.3961 | -0.0134 |
| C16 | C17 | 1.3947 | -0.0154 |
| C17 | C18 | 1.3962 | -0.0059 |

**Table S38.** B3PW91-GD3BJ calculated bond angles and differences for Compound **11**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C1 | Sn1 | C13 | 122.5 | 14.0 |
| C1 | Sn1 | N1 | 75.4 | 2.8 |
| C13 | Sn1 | N1 | 90.5 | 5.0 |
| C1 | Sn1 | Br2 | 119.0 | -7.6 |
| C13 | Sn1 | Br2 | 113.7 | -2.9 |
| N1 | Sn1 | Br2 | 82.6 | 2.1 |
| C1 | Sn1 | Br1 | 97.5 | 0.5 |
| N1 | Sn1 | Br1 | 170.7 | 2.2 |
| Br2 | Sn1 | Br1 | 96.0 | -4.8 |
| C8 | O1 | C10 | 106.4 | 0.9 |
| C8 | N1 | C9 | 108.0 | 1.0 |
| C8 | N1 | Sn1 | 117.0 | 0.6 |
| C9 | N1 | Sn1 | 131.9 | -0.7 |
| C2 | C1 | Sn1 | 111.4 | 1.0 |
| C3 | C2 | C7 | 117.8 | 0.5 |
| C3 | C2 | C1 | 119.6 | -0.7 |
| C7 | C2 | C1 | 122.6 | 0.2 |
| C4 | C3 | C2 | 121.6 | -0.3 |
| C5 | C4 | C3 | 120.3 | 0.0 |
| C4 | C5 | C6 | 119.3 | 0.9 |
| C5 | C6 | C7 | 120.7 | -0.7 |
| C2 | C7 | C6 | 120.4 | -0.4 |
| C2 | C7 | C8 | 121.4 | 0.4 |
| C6 | C7 | C8 | 118.1 | 0.1 |
| N1 | C8 | O1 | 116.3 | -0.2 |
| N1 | C8 | C7 | 127.5 | 1.0 |
| O1 | C8 | C7 | 116.2 | -0.9 |
| N1 | C9 | C11 | 108.4 | 1.9 |
| N1 | C9 | C12 | 112.4 | -1.9 |
| C11 | C9 | C12 | 111.2 | 0.7 |
| N1 | C9 | C10 | 101.6 | 0.4 |
| C11 | C9 | C10 | 111.5 | -0.5 |
| C12 | C9 | C10 | 111.3 | -0.6 |
| O1 | C10 | C9 | 104.4 | 1.1 |
| C18 | C13 | C14 | 119.2 | 0.2 |
| C18 | C13 | Sn1 | 120.6 | 1.9 |
| C14 | C13 | Sn1 | 120.2 | -2.4 |
| C15 | C14 | C13 | 120.3 | -0.2 |
| C16 | C15 | C14 | 120.1 | -0.1 |
| C17 | C16 | C15 | 119.9 | 0.4 |
| C16 | C17 | C18 | 119.9 | 0.0 |
| C13 | C18 | C17 | 120.5 | -0.3 |

**Table S39**. PBE0-GD3BJ calculated bond lengths and differences for Compound **11**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1 | C1 | 2.1475 | -0.0212 |
| Sn1 | C13 | 2.1213 | 0.0091 |
| Sn1 | N1 | 2.4942 | -0.0695 |
| Sn1 | Br2 | 2.5257 | -0.0090 |
| Sn1 | Br1 | 2.5857 | 0.0537 |
| O1 | C8 | 1.3454 | 0.0006 |
| O1 | C10 | 1.4364 | -0.0007 |
| N1 | C8 | 1.2908 | -0.0010 |
| N1 | C9 | 1.4834 | -0.0004 |
| C1 | C2 | 1.4867 | 0.0066 |
| C2 | C3 | 1.3994 | -0.0101 |
| C2 | C7 | 1.4128 | -0.0098 |
| C3 | C4 | 1.3901 | -0.0045 |
| C4 | C5 | 1.3943 | -0.0241 |
| C5 | C6 | 1.3870 | -0.0076 |
| C6 | C7 | 1.4022 | 0.0053 |
| C7 | C8 | 1.4607 | 0.0047 |
| C9 | C11 | 1.5281 | -0.0092 |
| C9 | C12 | 1.5216 | -0.0023 |
| C9 | C10 | 1.5397 | 0.0029 |
| C13 | C18 | 1.3984 | -0.0104 |
| C13 | C14 | 1.3987 | -0.0045 |
| C14 | C15 | 1.3935 | -0.0067 |
| C15 | C16 | 1.3946 | -0.0119 |
| C16 | C17 | 1.3933 | -0.0140 |
| C17 | C18 | 1.3950 | -0.0048 |

**Table S40.** PBE0-GD3BJ calculated bond angles and differences for Compound **11**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C1 | Sn1 | C13 | 122.0 | 14.5 |
| C1 | Sn1 | N1 | 75.0 | 3.2 |
| C13 | Sn1 | N1 | 90.4 | 5.0 |
| C1 | Sn1 | Br2 | 119.6 | -8.2 |
| C13 | Sn1 | Br2 | 113.5 | -2.7 |
| N1 | Sn1 | Br2 | 82.8 | 1.8 |
| C1 | Sn1 | Br1 | 97.5 | 0.5 |
| N1 | Sn1 | Br1 | 170.4 | 2.5 |
| Br2 | Sn1 | Br1 | 96.0 | -4.9 |
| C8 | O1 | C10 | 106.3 | 1.0 |
| C8 | N1 | C9 | 107.7 | 1.2 |
| C8 | N1 | Sn1 | 117.2 | 0.4 |
| C9 | N1 | Sn1 | 132.4 | -1.1 |
| C2 | C1 | Sn1 | 112.1 | 0.2 |
| C3 | C2 | C7 | 117.7 | 0.5 |
| C3 | C2 | C1 | 119.6 | -0.6 |
| C7 | C2 | C1 | 122.7 | 0.1 |
| C4 | C3 | C2 | 121.6 | -0.3 |
| C5 | C4 | C3 | 120.3 | 0.0 |
| C4 | C5 | C6 | 119.3 | 1.0 |
| C5 | C6 | C7 | 120.7 | -0.7 |
| C2 | C7 | C6 | 120.4 | -0.5 |
| C2 | C7 | C8 | 121.5 | 0.3 |
| C6 | C7 | C8 | 118.0 | 0.2 |
| N1 | C8 | O1 | 116.4 | -0.3 |
| N1 | C8 | C7 | 127.6 | 0.9 |
| O1 | C8 | C7 | 116.0 | -0.6 |
| N1 | C9 | C11 | 108.5 | 1.8 |
| N1 | C9 | C12 | 112.5 | -1.9 |
| C11 | C9 | C12 | 111.1 | 0.7 |
| N1 | C9 | C10 | 101.7 | 0.3 |
| C11 | C9 | C10 | 111.4 | -0.4 |
| C12 | C9 | C10 | 111.3 | -0.6 |
| O1 | C10 | C9 | 104.4 | 1.2 |
| C18 | C13 | C14 | 119.1 | 0.2 |
| C18 | C13 | Sn1 | 120.5 | 2.0 |
| C14 | C13 | Sn1 | 120.3 | -2.5 |
| C15 | C14 | C13 | 120.4 | -0.2 |
| C16 | C15 | C14 | 120.1 | -0.1 |
| C17 | C16 | C15 | 119.9 | 0.4 |
| C16 | C17 | C18 | 119.9 | 0.0 |
| C13 | C18 | C17 | 120.5 | -0.3 |

**Table S41**. M05-2X-GD3 calculated bond lengths and differences for Compound **11**

| Calculated Bond Length (Å) | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|
| Sn1 | C1 | 2.1369 | -0.0106 |
| Sn1 | C13 | 2.1086 | 0.0218 |
| Sn1 | N1 | 2.4863 | -0.0616 |
| Sn1 | Br2 | 2.5292 | -0.0125 |
| Sn1 | Br1 | 2.5892 | 0.0502 |
| O1 | C8 | 1.3480 | -0.0020 |
| O1 | C10 | 1.4432 | -0.0074 |
| N1 | C8 | 1.2884 | 0.0015 |
| N1 | C9 | 1.4899 | -0.0068 |
| C1 | C2 | 1.4920 | 0.0013 |
| C2 | C3 | 1.3990 | -0.0097 |
| C2 | C7 | 1.4102 | -0.0072 |
| C3 | C4 | 1.3897 | -0.0042 |
| C4 | C5 | 1.3941 | -0.0240 |
| C5 | C6 | 1.3867 | -0.0073 |
| C6 | C7 | 1.4014 | 0.0061 |
| C7 | C8 | 1.4659 | -0.0005 |
| C9 | C11 | 1.5299 | -0.0110 |
| C9 | C12 | 1.5234 | -0.0040 |
| C9 | C10 | 1.5356 | 0.0069 |
| C13 | C18 | 1.3976 | -0.0097 |
| C13 | C14 | 1.3980 | -0.0038 |
| C14 | C15 | 1.3935 | -0.0066 |
| C15 | C16 | 1.3946 | -0.0119 |
| C16 | C17 | 1.3934 | -0.0140 |
| C17 | C18 | 1.3949 | -0.0046 |

**Table S42.** M05-2X-GD3 calculated bond angles and differences for Compound **11**

| Calculated Bond Angle (°) | | | | Differences in Bond Length (Calc. – Exp.) |
|---|---|---|---|---|
| C1 | Sn1 | C13 | 122.2 | 14.4 |
| C1 | Sn1 | N1 | 75.5 | 2.8 |
| C13 | Sn1 | N1 | 90.1 | 5.4 |
| C1 | Sn1 | Br2 | 119.7 | -8.4 |
| C13 | Sn1 | Br2 | 113.3 | -2.6 |
| N1 | Sn1 | Br2 | 83.1 | 1.6 |
| C1 | Sn1 | Br1 | 97.6 | 0.4 |
| N1 | Sn1 | Br1 | 170.8 | 2.1 |
| Br2 | Sn1 | Br1 | 95.4 | -4.2 |
| C8 | O1 | C10 | 106.0 | 1.4 |
| C8 | N1 | C9 | 107.4 | 1.5 |
| C8 | N1 | Sn1 | 116.1 | 1.5 |
| C9 | N1 | Sn1 | 132.9 | -1.7 |
| C2 | C1 | Sn1 | 111.7 | 0.7 |
| C3 | C2 | C7 | 117.7 | 0.5 |
| C3 | C2 | C1 | 119.4 | -0.5 |
| C7 | C2 | C1 | 122.9 | -0.1 |
| C4 | C3 | C2 | 121.5 | -0.2 |
| C5 | C4 | C3 | 120.3 | -0.1 |
| C4 | C5 | C6 | 119.3 | 1.0 |
| C5 | C6 | C7 | 120.6 | -0.6 |
| C2 | C7 | C6 | 120.6 | -0.6 |
| C2 | C7 | C8 | 121.5 | 0.3 |
| C6 | C7 | C8 | 117.8 | 0.4 |
| N1 | C8 | O1 | 116.3 | -0.1 |
| N1 | C8 | C7 | 127.8 | 0.7 |
| O1 | C8 | C7 | 115.9 | -0.5 |
| N1 | C9 | C11 | 108.4 | 1.9 |
| N1 | C9 | C12 | 113.1 | -2.6 |
| C11 | C9 | C12 | 111.2 | 0.6 |
| N1 | C9 | C10 | 101.4 | 0.6 |
| C11 | C9 | C10 | 111.0 | 0.1 |
| C12 | C9 | C10 | 111.4 | -0.7 |
| O1 | C10 | C9 | 103.7 | 1.9 |
| C18 | C13 | C14 | 119.2 | 0.2 |
| C18 | C13 | Sn1 | 120.5 | 2.0 |
| C14 | C13 | Sn1 | 120.3 | -2.5 |
| C15 | C14 | C13 | 120.3 | -0.2 |
| C16 | C15 | C14 | 120.1 | -0.1 |
| C17 | C16 | C15 | 120.0 | 0.3 |
| C16 | C17 | C18 | 119.8 | 0.1 |
| C13 | C18 | C17 | 120.5 | -0.3 |