

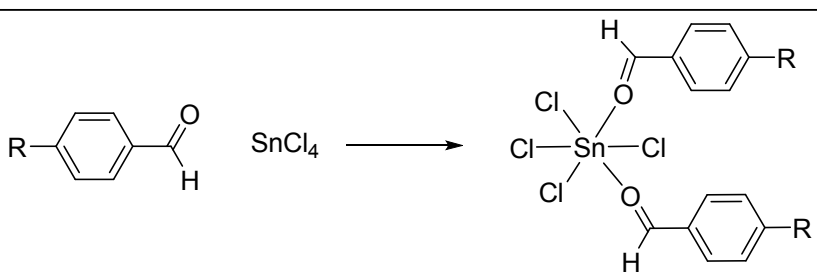
Electronic Supporting Information-ES1

**Triggering the approach of an Arene or Heteroarene
towards an aldehyde *via* Lewis acid-aldehyde
communication**

Sanjay Pratihar *

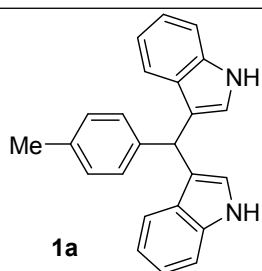
Department of chemical Sciences, Tezpur University, Napaam, Asaam-784028

Table S1. Difference in bond order of aldehyde after the coordination with SnCl₄

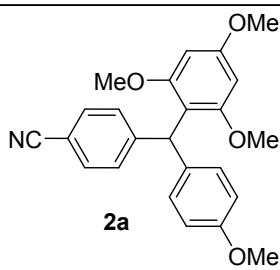


Bond order	CHO-Sn	CO (free aldehyde)	CO (complex)	Δ CO (free-complex)	Sn-Cl (trans)	Sn-Cl (cis)
R = OMe	0.275	1.883	1.569	0.314	0.670	0.690
R = Me	0.266	1.894	1.595	0.299	0.677	0.694
R = H	0.260	1.900	1.611	0.289	0.681	0.698
R = Cl	0.256	1.902	1.612	0.290	0.684	0.699
R = CF ₃	0.247	1.910	1.633	0.277	0.692	0.702
R = CN	0.243	1.911	1.638	0.273	0.693	0.706

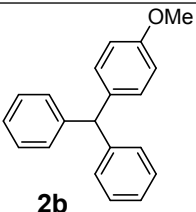
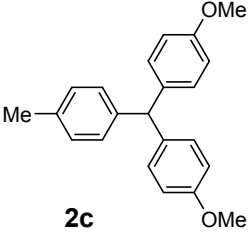
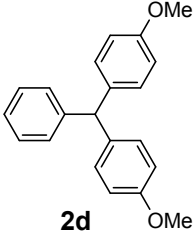
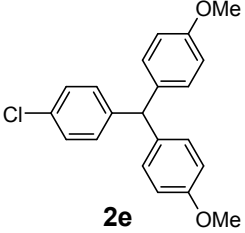
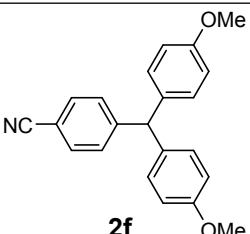
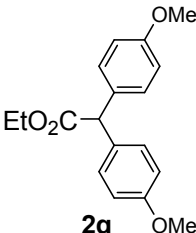
S1.2 Spectral and Analytical Data



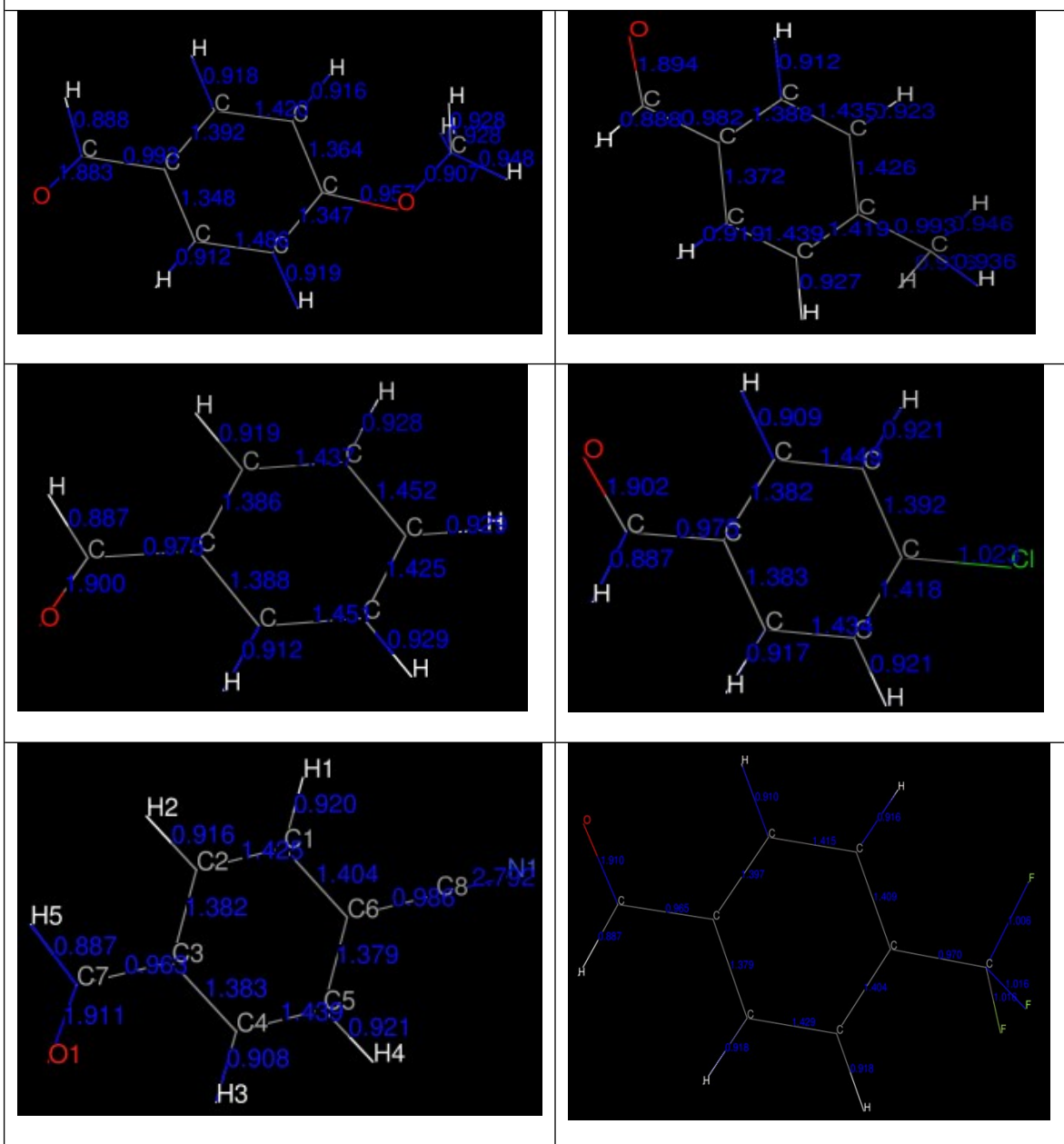
$\delta_{\text{H}}(\text{CDCl}_3)$ 2.36 (3H, s), 5.87 (1H, s), 6.59 (2H, d, $J = 2.0$ Hz), 6.99-7.34 (10H, m), 7.43 (2H, d, $J = 7.8$ Hz), 7.78 (2H, s).
 $\delta_{\text{C}}(\text{CDCl}_3)$ 21.1, 39.8, 111.1, 119.2, 119.8, 120.0, 121.9, 123.6, 127.1, 128.6, 128.9, 135.5, 136.7, 141.1.

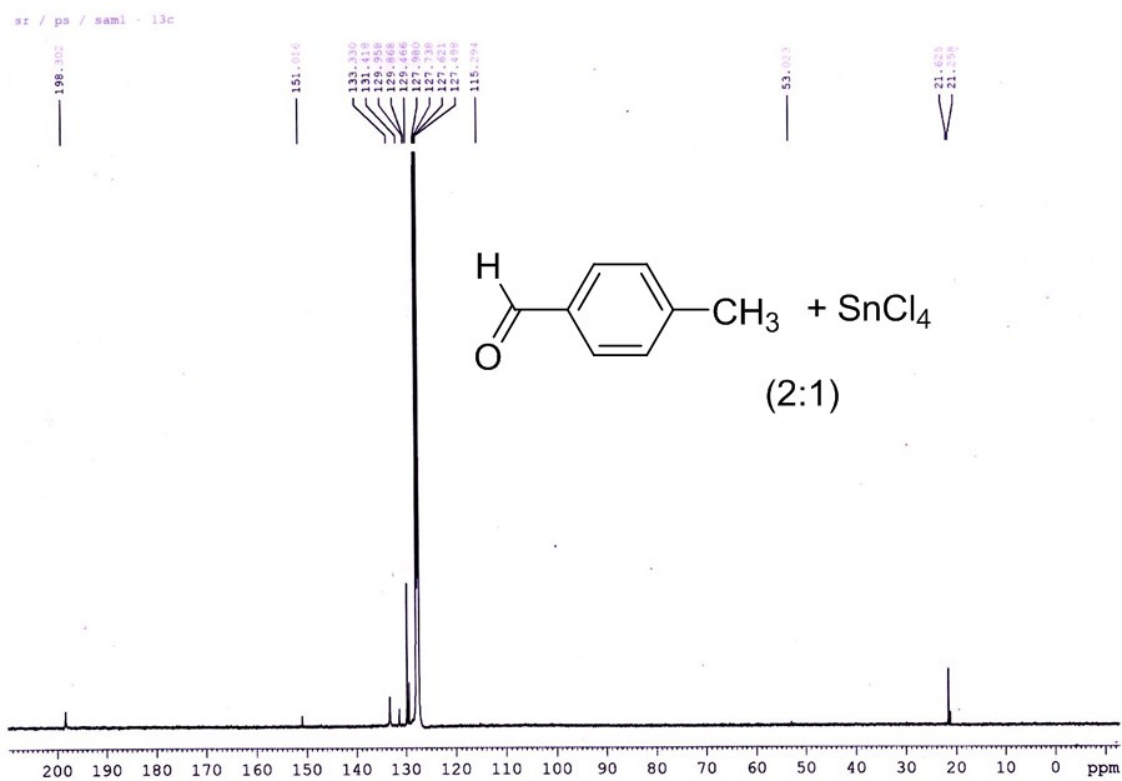
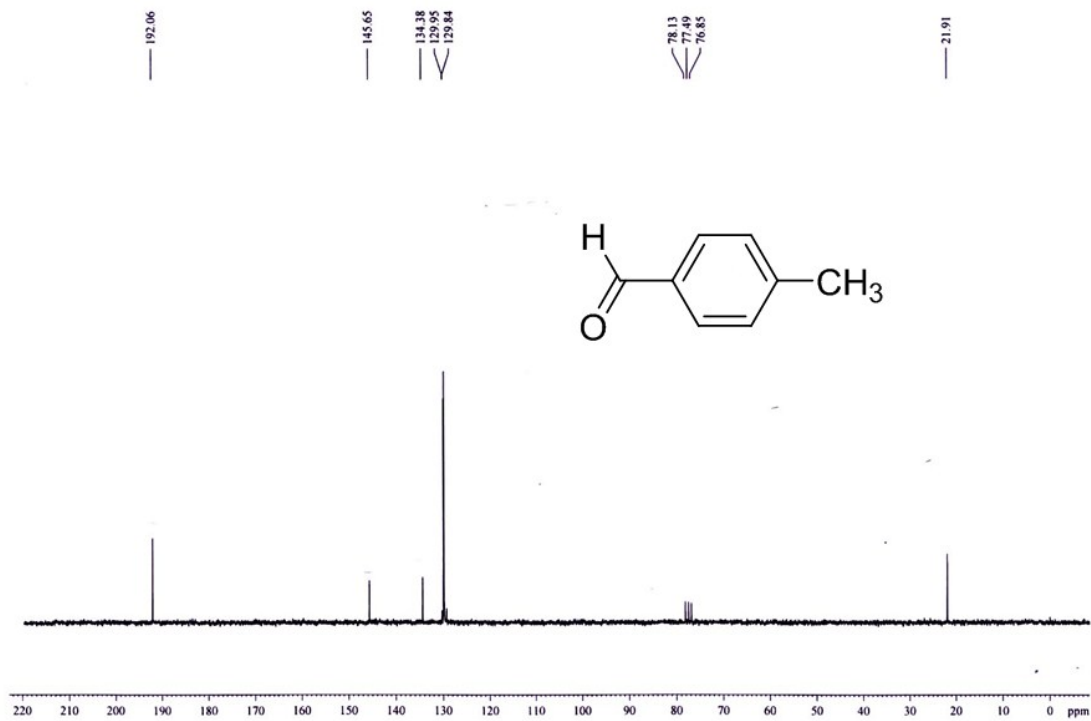


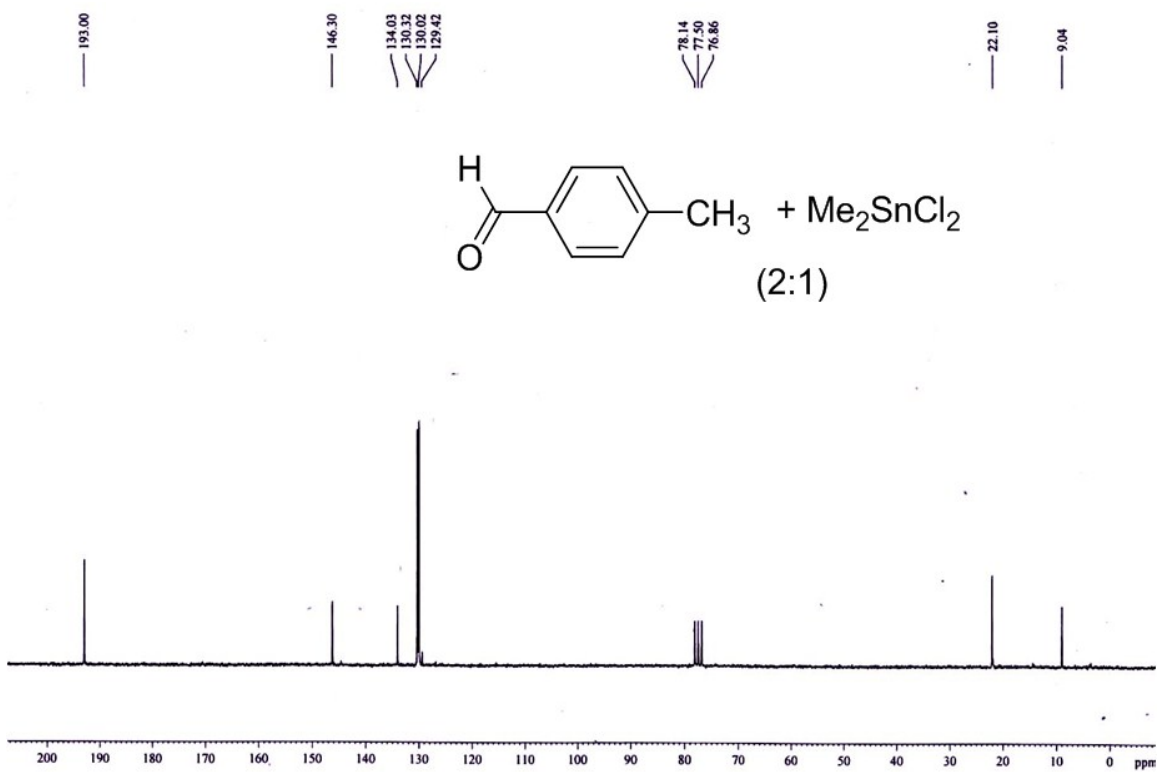
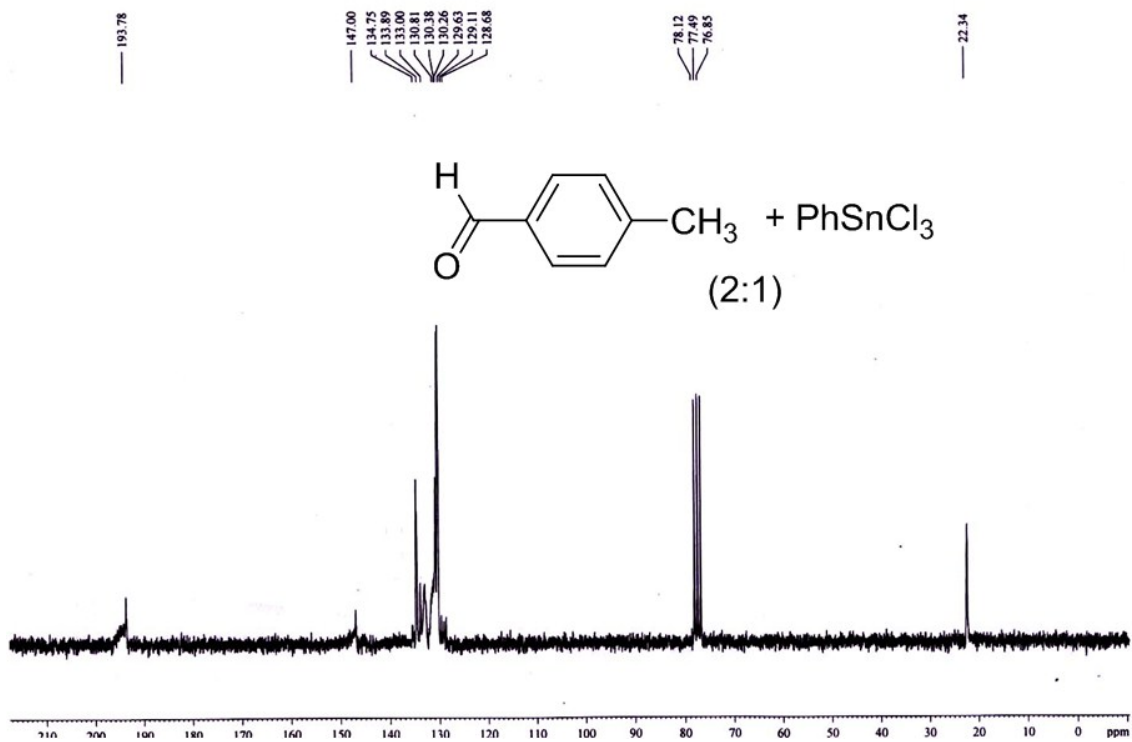
$\delta_{\text{H}}(\text{CDCl}_3)$ 3.57 (3H, s), 3.75 (3H, s), 3.77 (3H, s), 5.96 (1H, s, CH), 6.11 (1H, s), 6.77 (2H, d, $J = 8.8$ Hz), 7.07 (2H, d, $J = 8.4$ Hz), 7.14 (2H, d, $J = 8.0$ Hz), 7.44 (2H, d, $J = 8.4$ Hz).
 $\delta_{\text{C}}(\text{CDCl}_3)$ 44.6, 55.2, 55.3, 55.5, 55.6, 91.5, 108.7, 112.4, 113.4, 119.5, 129.4, 130.2, 131.2, 134.1, 151.3, 157.9, 158.8, 160.4.

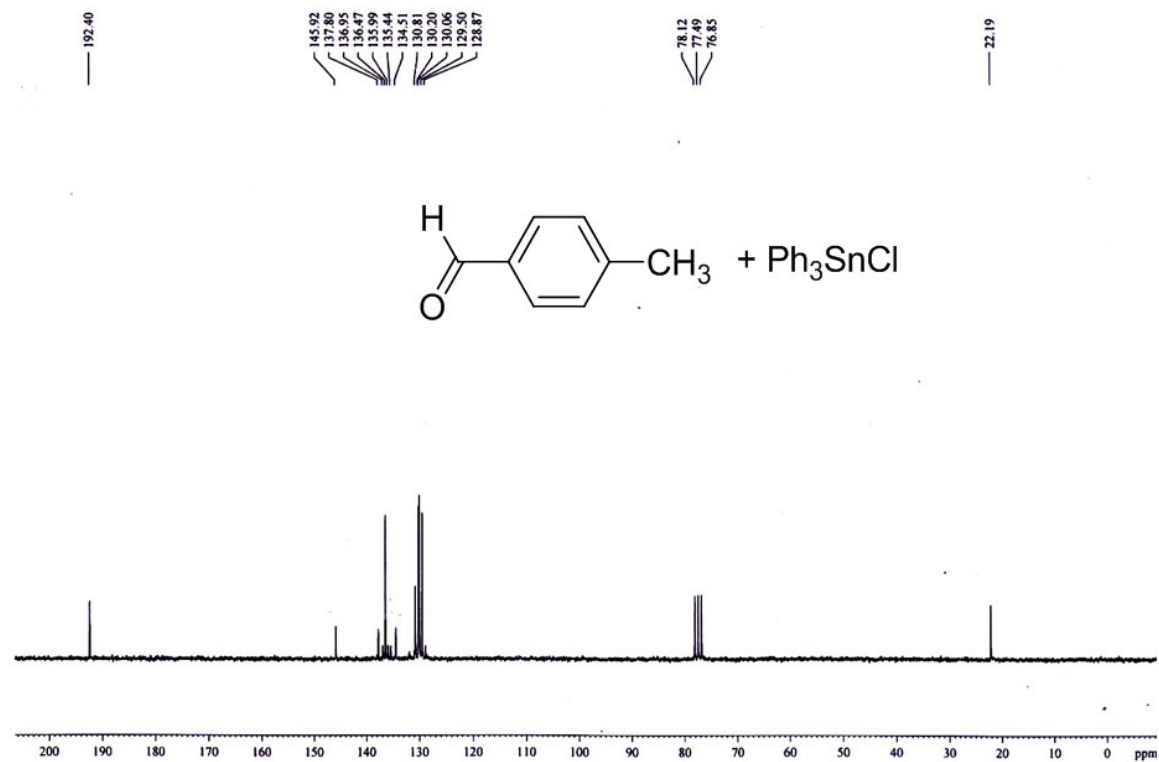
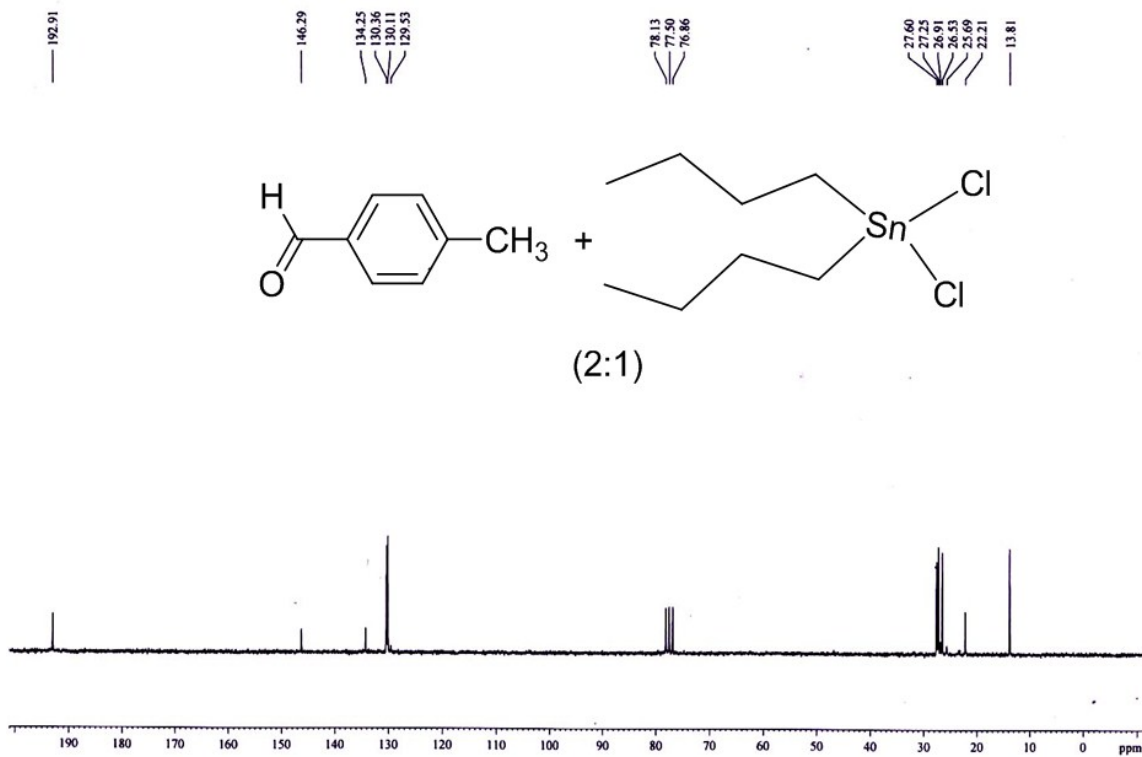
 <p>2b</p>	<p>HRMS (ESI) calcd for C₂₄H₂₃NO₄ [M+H]⁺ = 390.1705, found 390.1699.</p> <p>δ_{H}(CDCl₃) 3.79 (3H, s), 5.51 (1H, s, CH), 6.79-6.86 (2H, m), 7.0-7.33 (12H, m).</p> <p>δ_{C}(CDCl₃) 55.2, 56.1, 113.7, 126.2, 128.3, 129.4, 130.4, 136.1, 144.3, 158.1.</p>
 <p>2c</p>	<p>δ_{H}(CDCl₃) 2.33 (3H, s, CH₃), 3.79 (6H, s, 2 OCH₃), 5.43 (1H, s, CH), 6.80 (4H, d, <i>J</i> = 7.8 Hz, CH aromat.), 6.97-7.12 (8H, m, CH aromat.).</p> <p>δ_{C}(CDCl₃) 20.9, 54.6, 55.2, 113.6, 128.9, 129.2, 130.2, 135.6, 136.7, 141.6, 157.9.</p>
 <p>2d</p>	<p>δ_{H}(CDCl₃) 3.78 (6H, s, 2 OCH₃), 5.45 (1H, s, CH), 6.82 (4H, d, <i>J</i> = 8.7 Hz, CH aromat.), 7.02 (4H, d, <i>J</i> = 8.7 Hz, CH aromat.), 7.08-7.28 (5H, m, CH aromat.).</p> <p>δ_{C}(CDCl₃) 48.8, 55.2, 113.7, 126.2, 128.3, 129.3, 130.3, 136.5, 144.6, 158.0.</p>
 <p>2e</p>	<p>δ_{H}(CDCl₃) 3.79 (6H, s, 2 OCH₃), 5.42 (1H, s, CH), 6.82 (4H, d, <i>J</i> = 8.7 Hz, CH aromat.), 6.99 (4H, d, <i>J</i> = 8.7 Hz, CH aromat.), 7.03 (2H, d, <i>J</i> = 8.5 Hz, CH aromat.), 7.24 (2H, d, <i>J</i> = 8.5 Hz, CH aromat.).</p> <p>δ_{C}(CDCl₃) 54.5, 55.2, 113.7, 128.3, 130.2, 130.6, 131.9, 135.9, 143.2, 158.1.</p>
 <p>2f</p>	<p>δ_{H}(CDCl₃) 3.79 (3H, s), 5.49 (1H, s, CH), 6.84 (4H, d, <i>J</i> = 8.6 Hz, CH aromat.), 6.99 (4H, d, <i>J</i> = 8.8 Hz, CH aromat.), 7.23 (2H, d, <i>J</i> = 8.2 Hz, CH aromat.), 7.56 (2H, d, <i>J</i> = 8.2 Hz, CH aromat.).</p> <p>δ_{C}(CDCl₃) 53.3, 110.1, 114.0, 119.0, 130.1, 130.2, 132.1, 134.9, 150.3, 158.4</p> <p>Anal. (C₂₂H₁₉NO₂) calcd, C: 80.22; H: 5.81 found, C: 79.98, H: 5.65.</p>
 <p>2g</p>	<p>δ_{H}(CDCl₃) 1.24 (3H, t, <i>J</i> = 7.2 Hz), 3.77 (3H, s), 4.22 (2H, q, <i>J</i> = 4.0 Hz), 4.90 (1H, s), 6.84 (4H, d, <i>J</i> = 8.8 Hz), 7.25 (4H, d, <i>J</i> = 8.8 Hz).</p> <p>δ_{C}(CDCl₃) 14.2, 55.2, 55.5, 61.1, 113.9, 129.5, 131.3, 158.7, 173.0. Anal. (C₂₀H₁₈O₄) calcd, C: 71.98; H: 6.71</p>

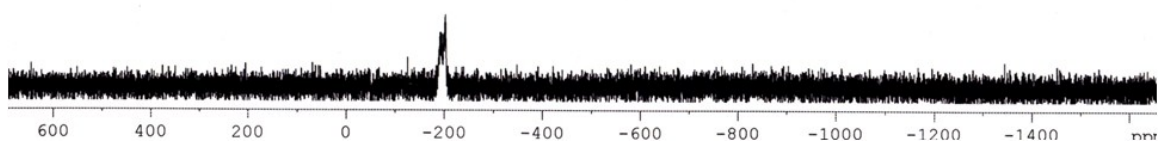
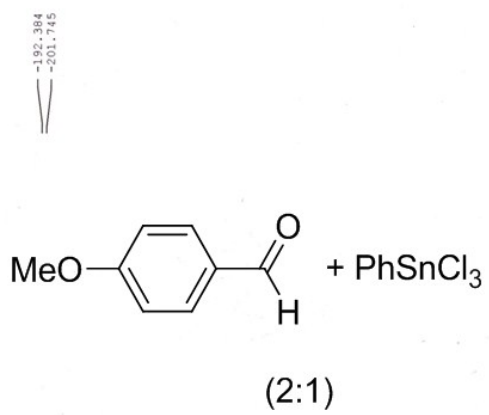
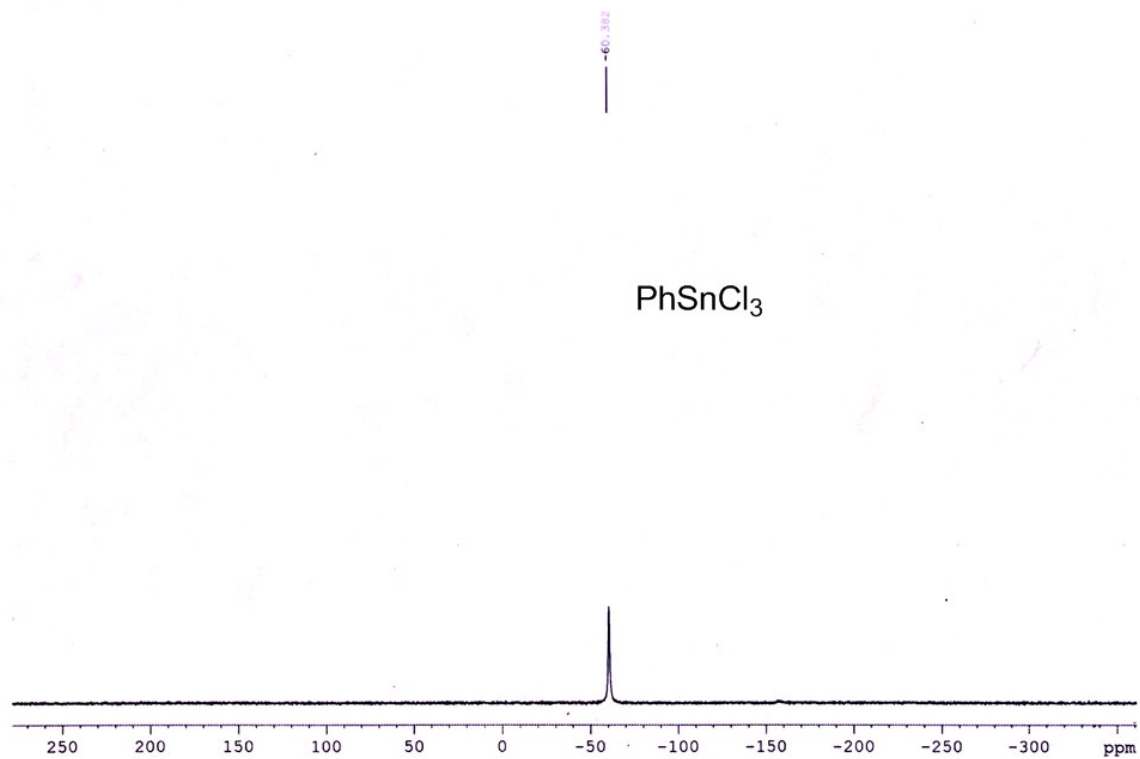
found, C: 71.72, H: 6.62.

Table S4. Bond order of six *para* substituted benzaldehyde.

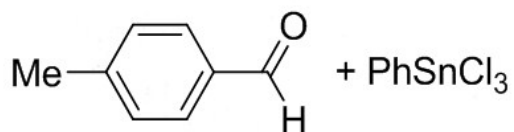




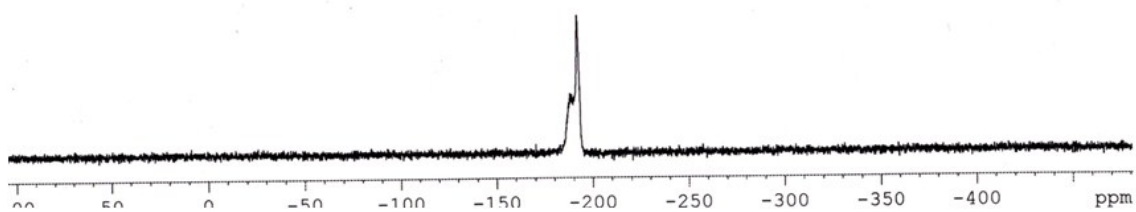




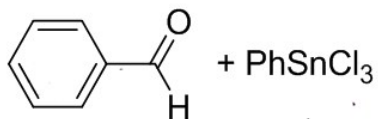
-188.188
-192.097



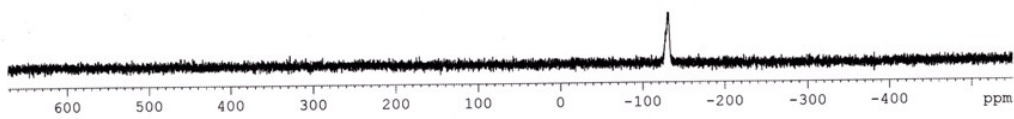
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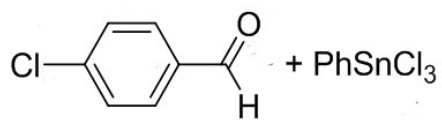
-131.960



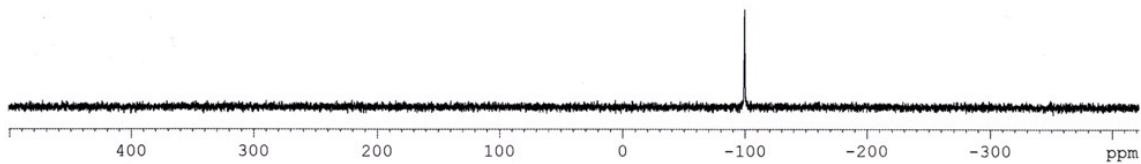
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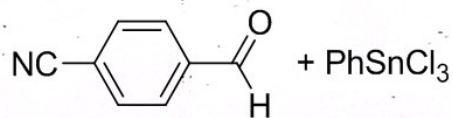
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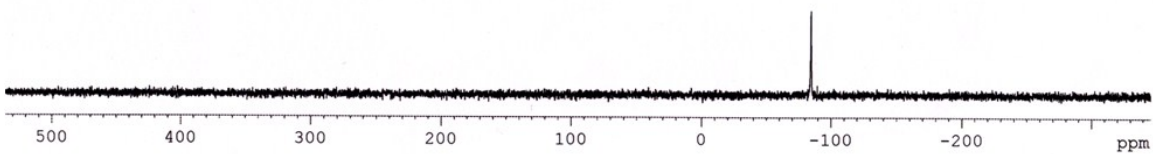
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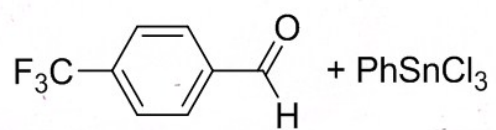
-84.471



(2:1)



-85.939



(2:1)

