

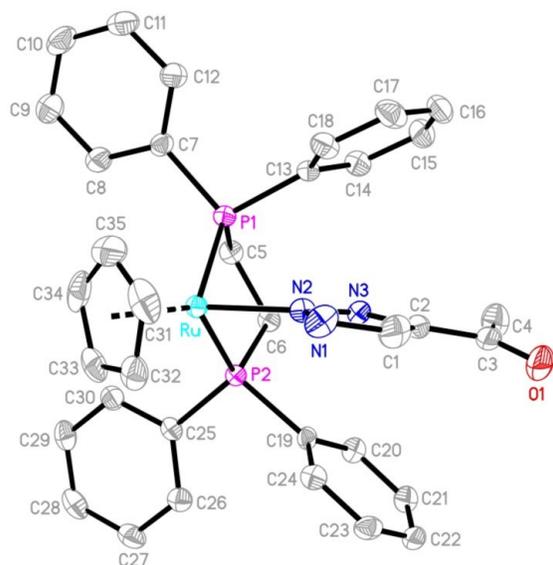
## Supporting Information

### The straightforwardly synthesis of N-coordinated ruthenium 4-aryl-1,2,3-triazolato complexes by [3+2] cycloaddition reactions of a ruthenium azido complex with terminal phenylacetylenes and non-covalent aromatic interactions in structures

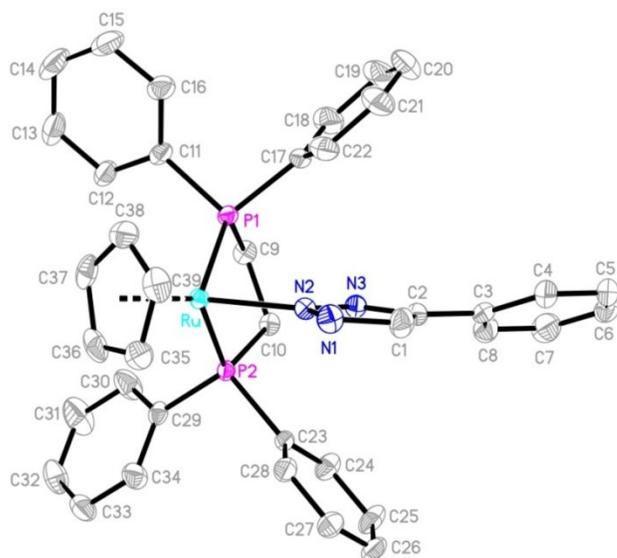
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#### Content:

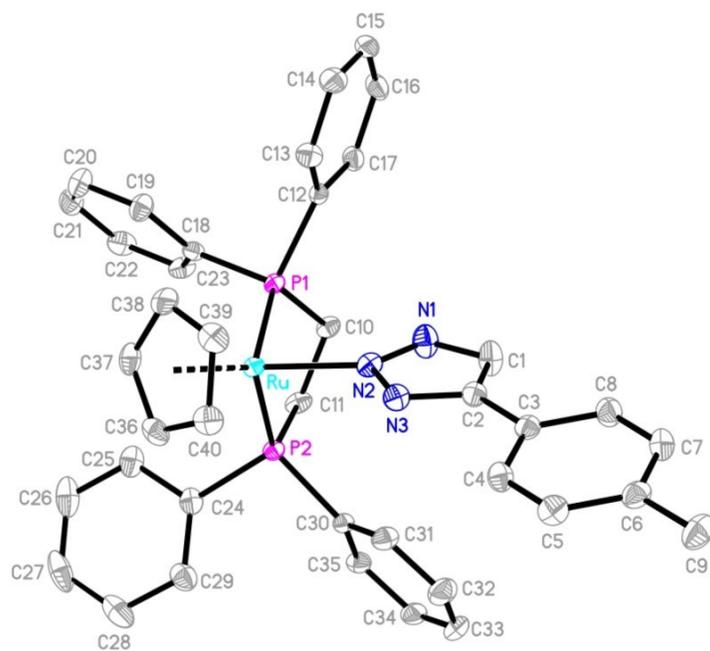
1. **Fig. S1** ORTEP drawing of **3**
2. **Fig. S2** ORTEP drawing of **5**
3. **Fig. S3** ORTEP drawing of **6**
4. **Fig. S4** Selected  $\pi\cdots\pi$  and aromatic C-H $\cdots\pi$  interactions of **3**
5. NMR spectra of all relevant compounds
6. IR spectra of compounds **2-6**



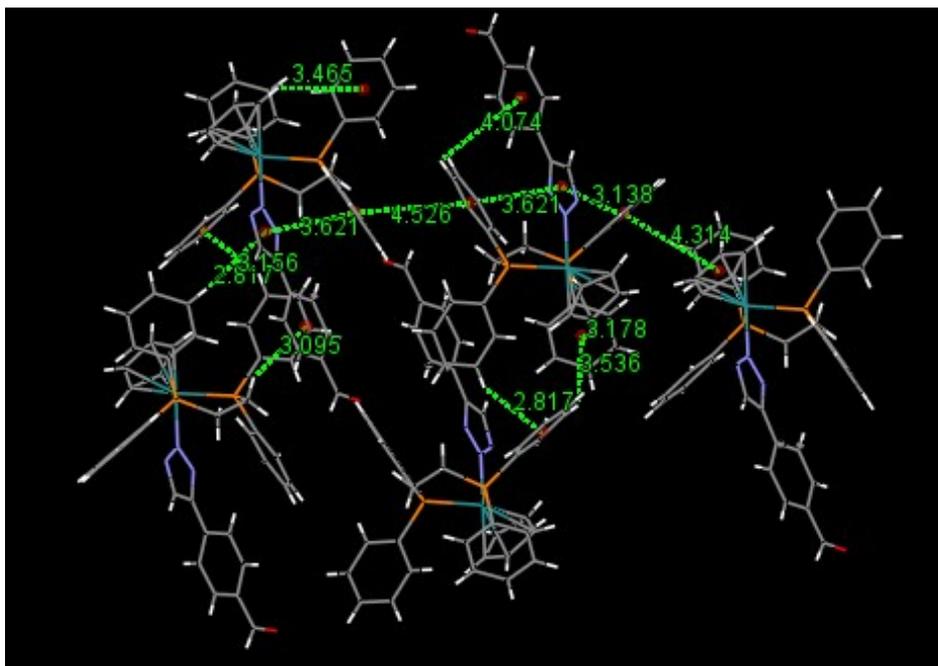
**Fig. S1** An ORTEP drawing of **3** with thermal ellipsoids shown at a 50% probability level. Hydrogen atoms have been omitted for clarity.



**Fig. S2** An ORTEP drawing of **5** with thermal ellipsoids shown at a 50% probability level. Hydrogen atoms and solvate  $\text{CHCl}_3$  have been omitted for clarity.



**Fig. S3** An ORTEP drawing of **6** with thermal ellipsoids shown at a 50% probability level. Hydrogen atoms have been omitted for clarity.



**Fig. S4** Selected  $\pi\cdots\pi$  and aromatic C-H $\cdots\pi$  interactions in the packing of **3**.

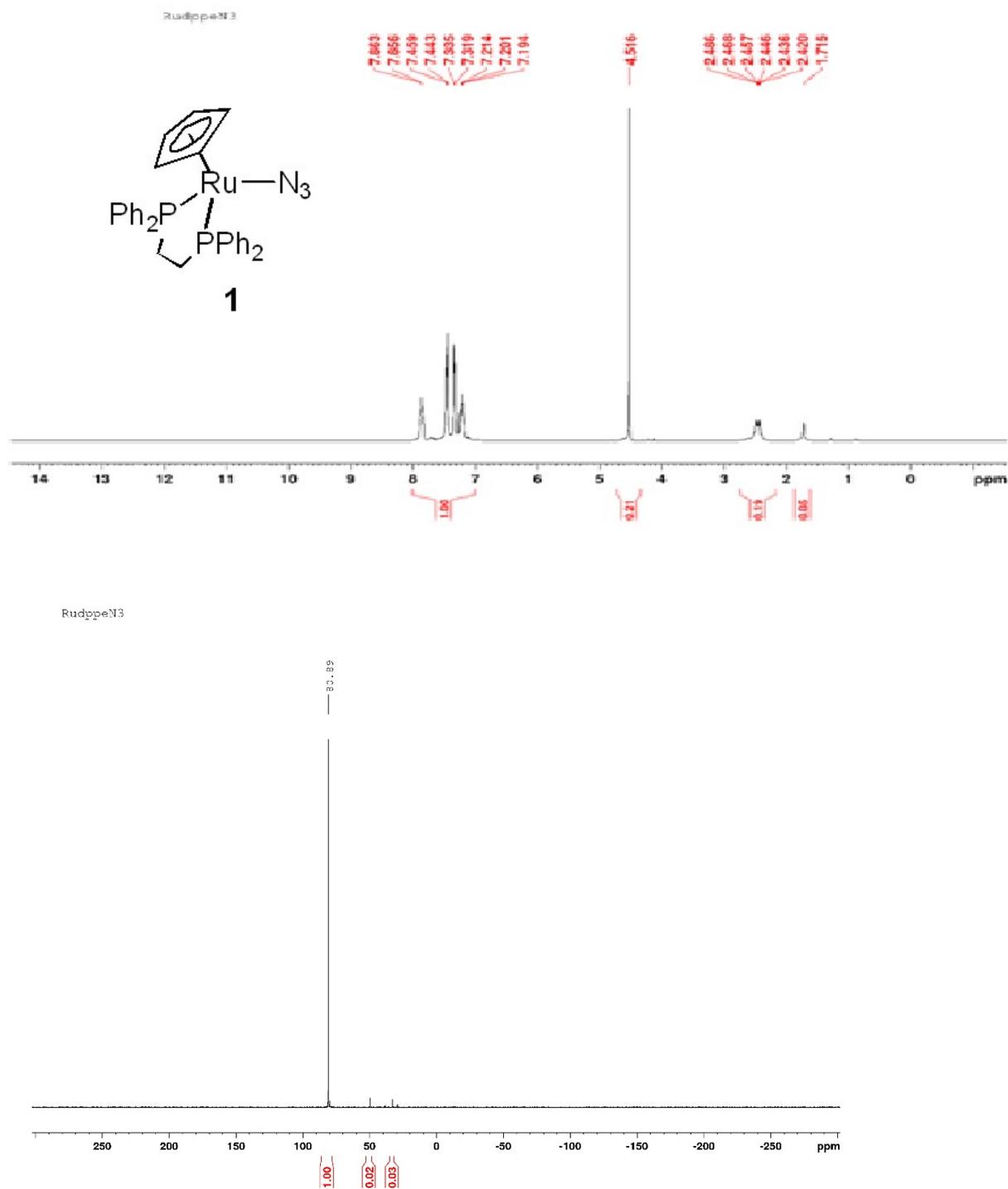
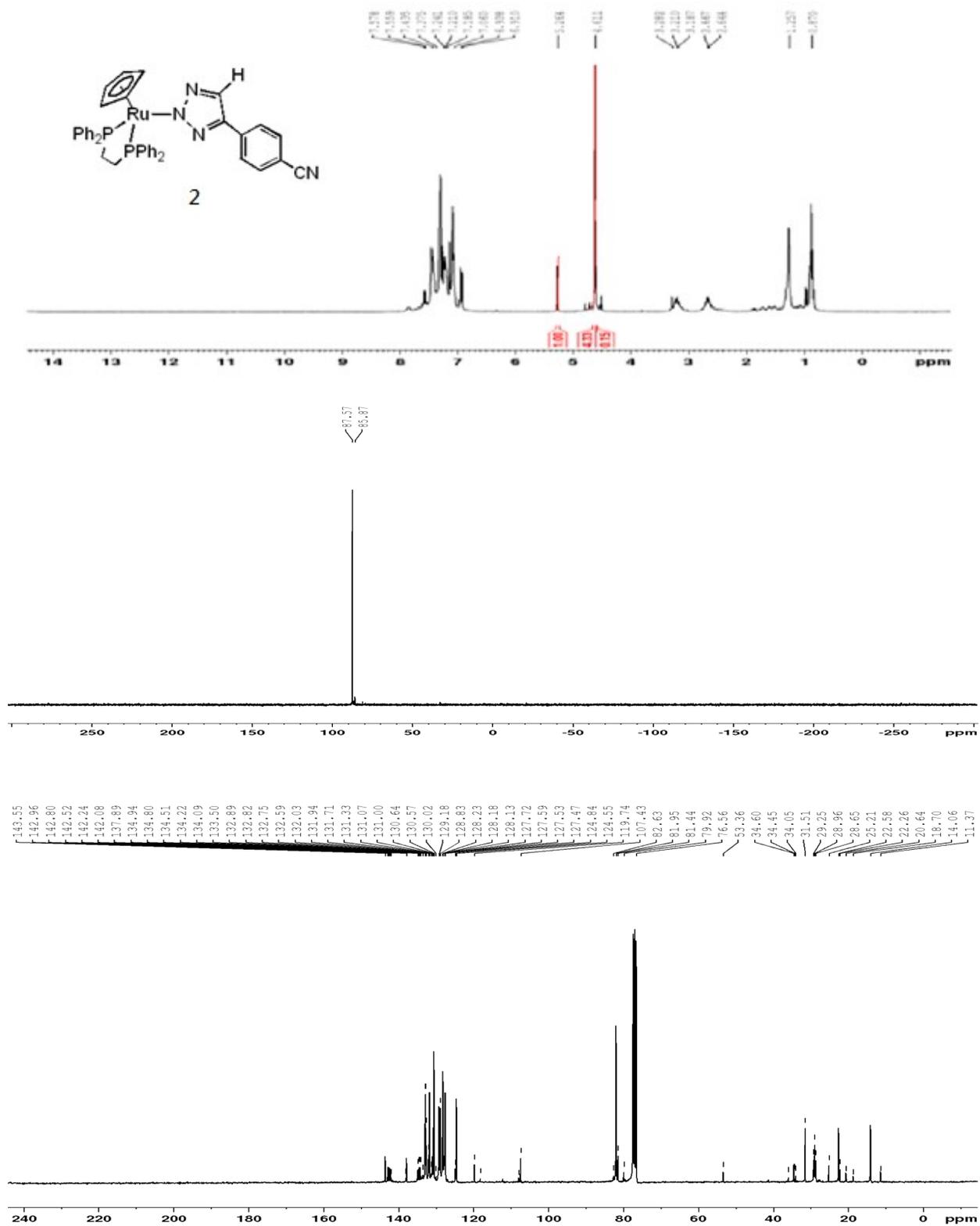


Fig. S5  $^1\text{H}$  NMR and  $^{31}\text{P}$  NMR spectra of compound **1**, [Ru]-N3.



**Fig. S6**  $^1\text{H}$ ,  $^{31}\text{P}$  and  $^{13}\text{C}$  NMR spectra of compound **2**,  $[\text{Ru}]_3\text{N}_3\text{C}_2\text{H}(4\text{-C}_6\text{H}_4\text{CN})$ .

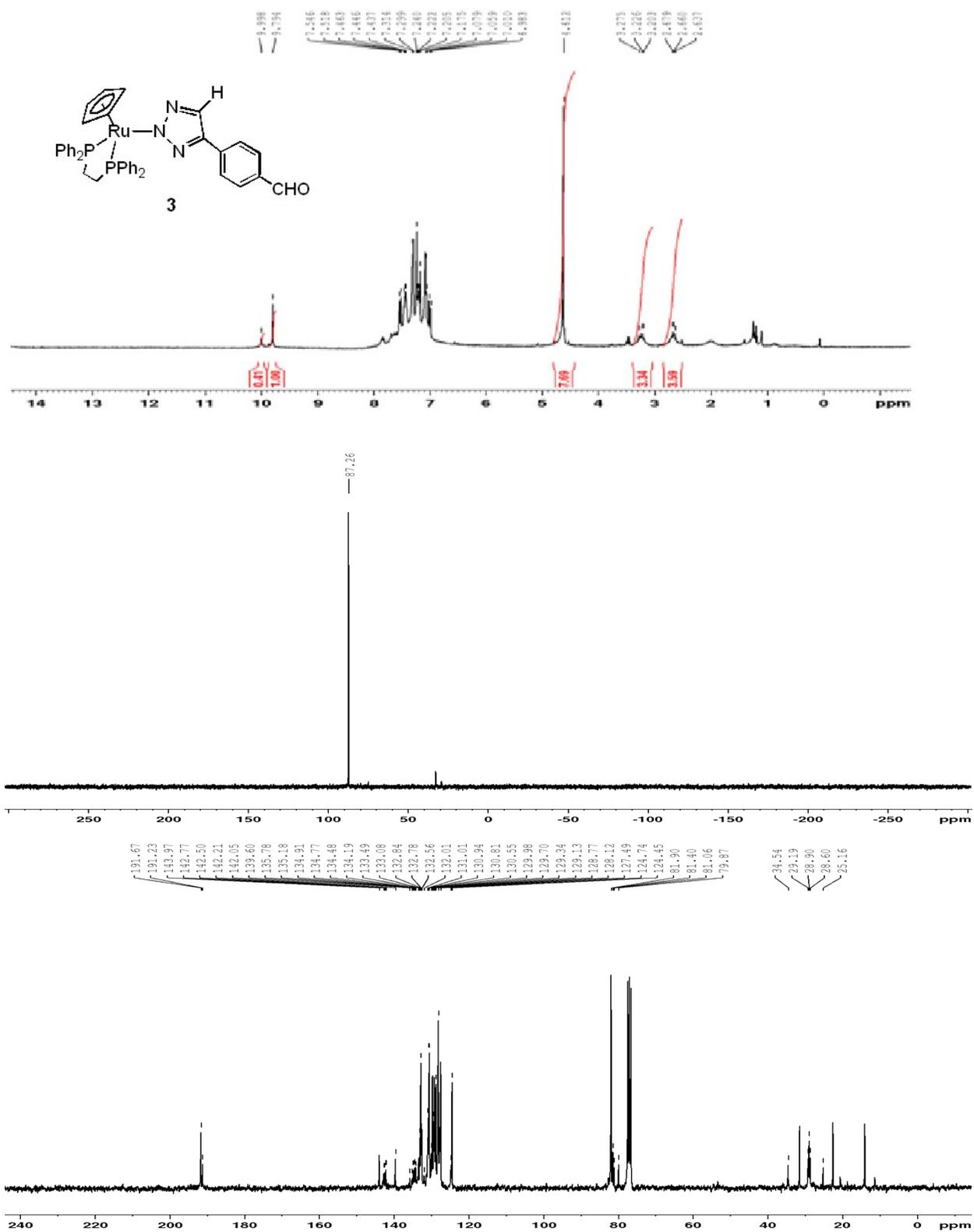


Fig. S7 <sup>1</sup>H, <sup>31</sup>P and <sup>13</sup>C NMR spectra of compound **3**, [Ru]N<sub>3</sub>C<sub>2</sub>H(4-C<sub>6</sub>H<sub>4</sub>CHO).

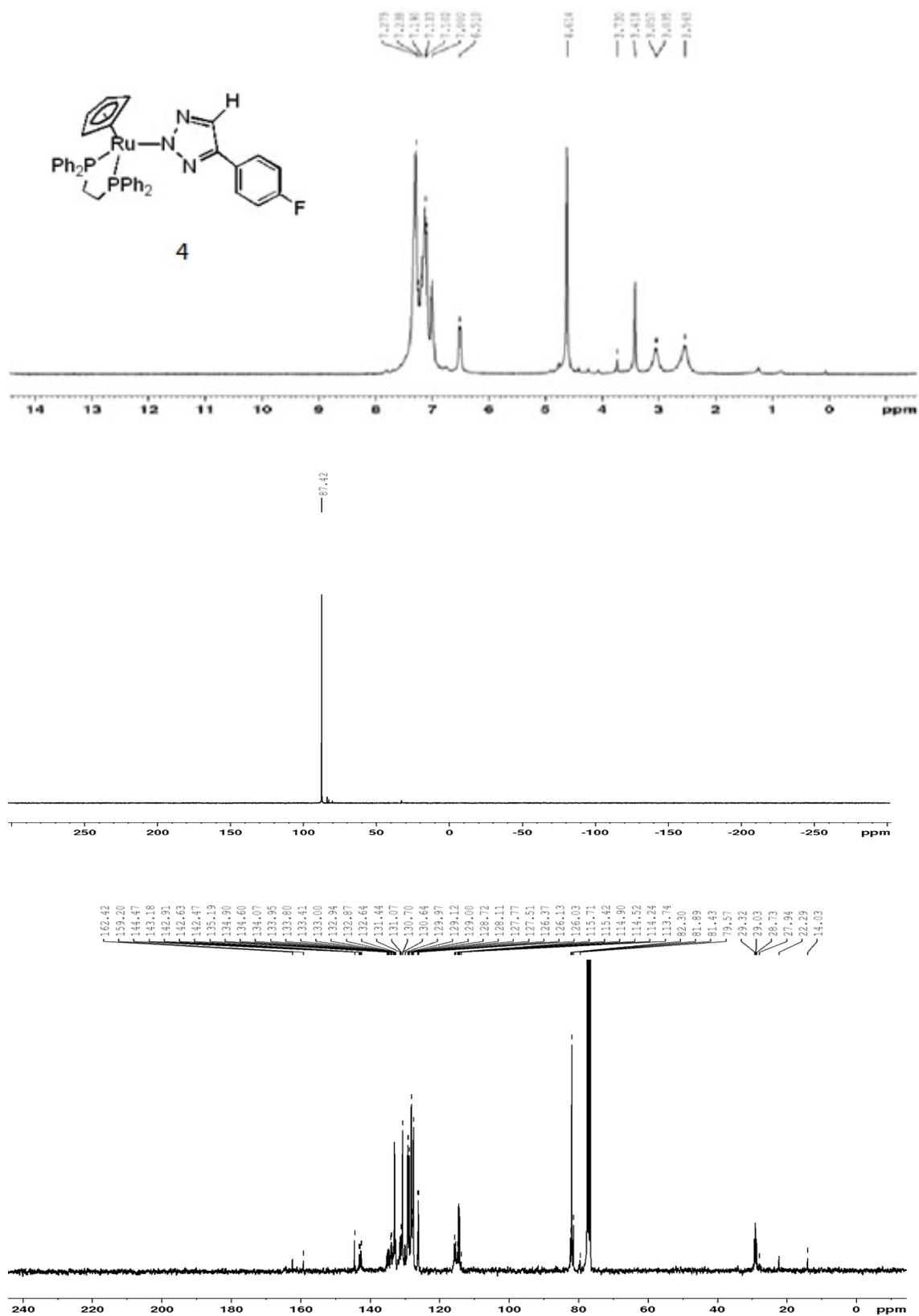


Fig. S8 <sup>1</sup>H, <sup>31</sup>P and <sup>13</sup>C NMR spectra of compound **4**, [Ru]N<sub>3</sub>C<sub>2</sub>H(4-C<sub>6</sub>H<sub>4</sub>F).

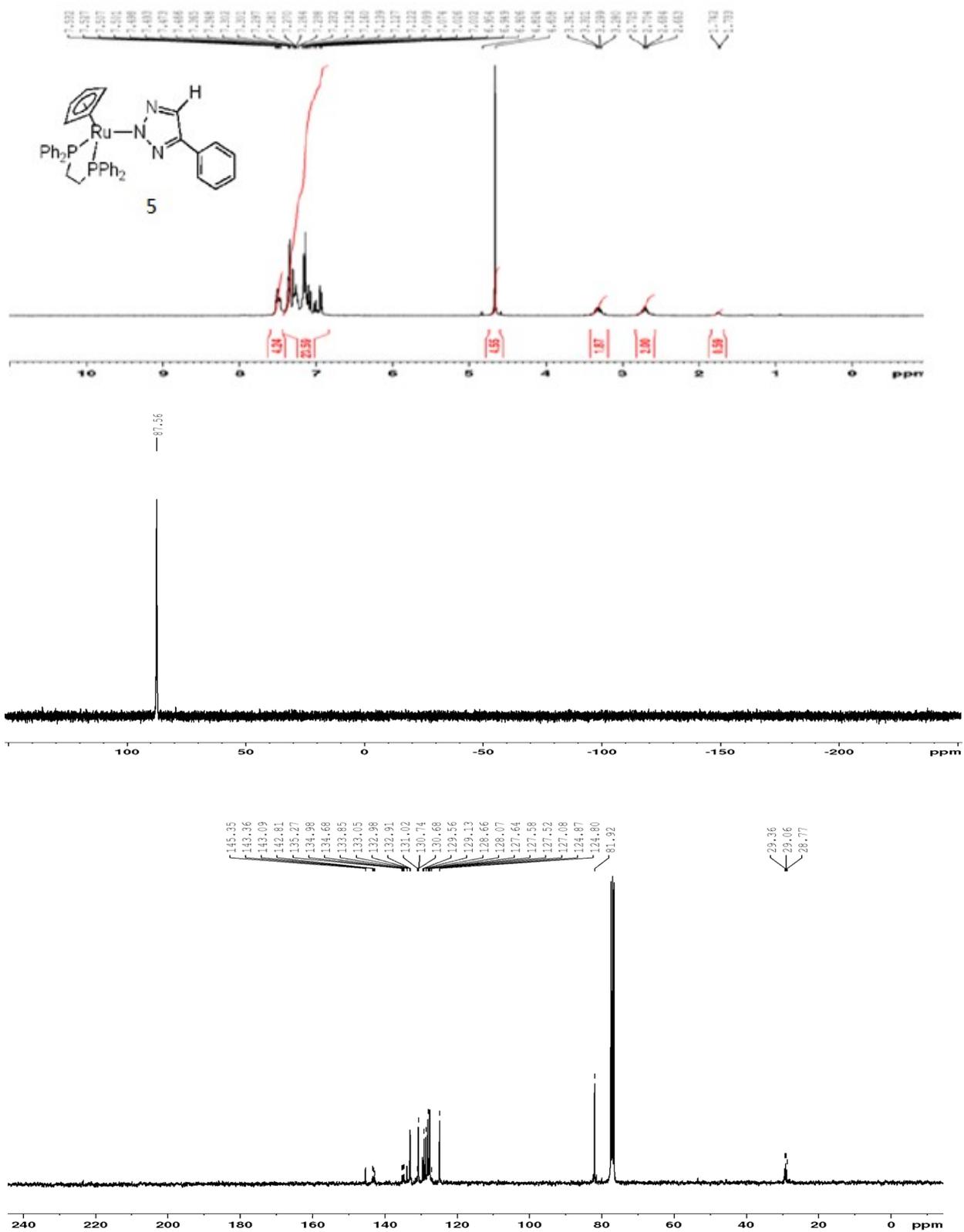
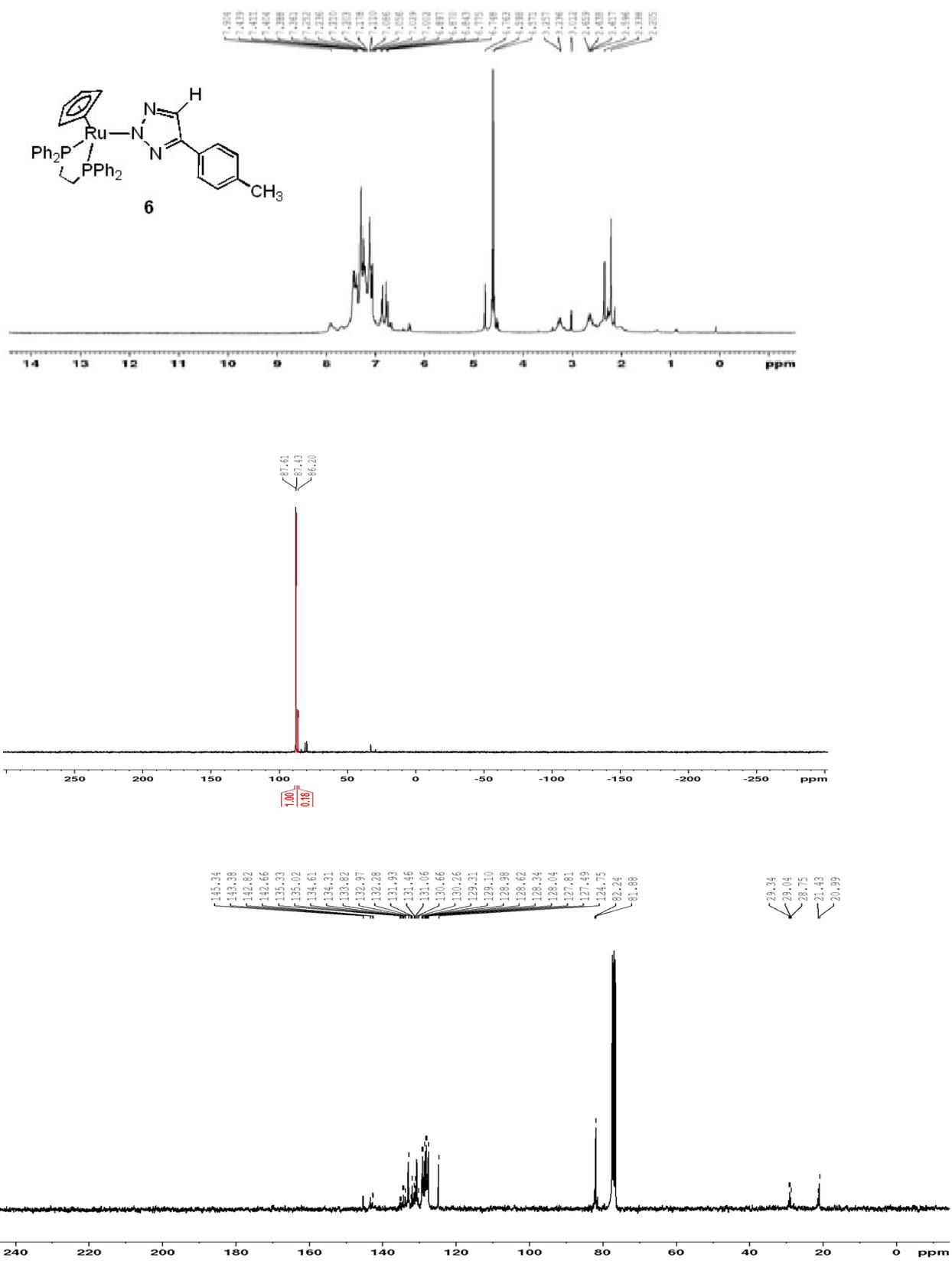


Fig. S9  $^1\text{H}$ ,  $^{31}\text{P}$  and  $^{13}\text{C}$  NMR spectra of compound 5  $[\text{Ru}]_3\text{N}_3\text{C}_2\text{HPh}$ .



**Fig. S10** <sup>1</sup>H, <sup>31</sup>P and <sup>13</sup>C NMR spectra of compound **6**, [Ru]N<sub>3</sub>C<sub>2</sub>H(4-C<sub>6</sub>H<sub>4</sub>CH<sub>3</sub>).

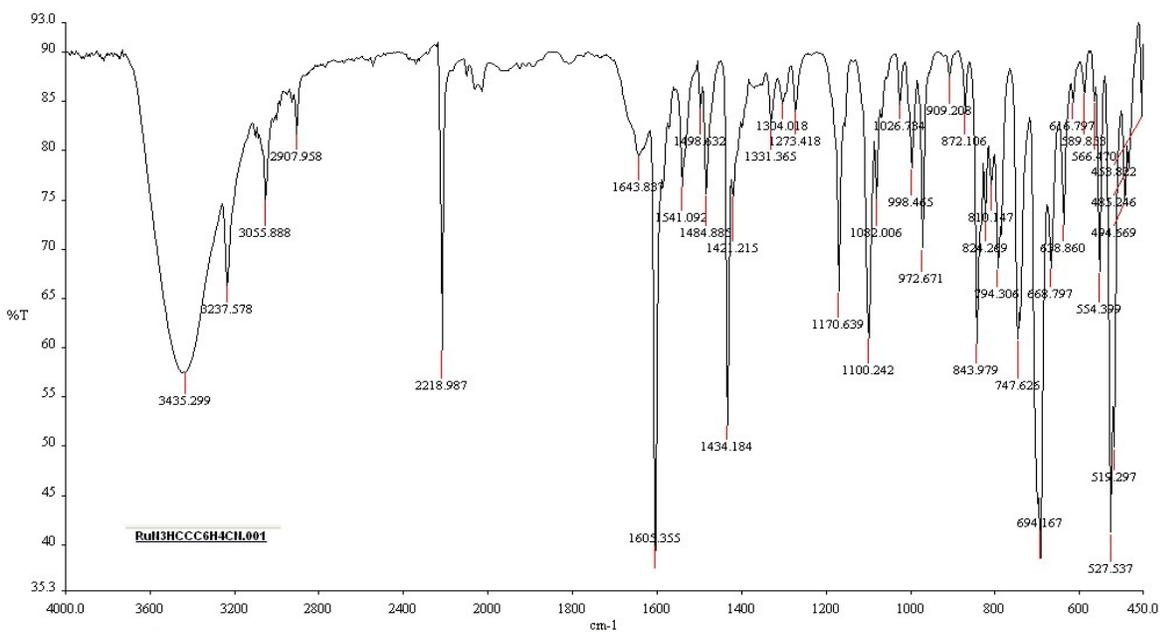


Fig. S11 IR spectra of compound 2,  $[\text{Ru}]\text{N}_3\text{C}_2\text{H}(4\text{-C}_6\text{H}_4\text{CN})$ .

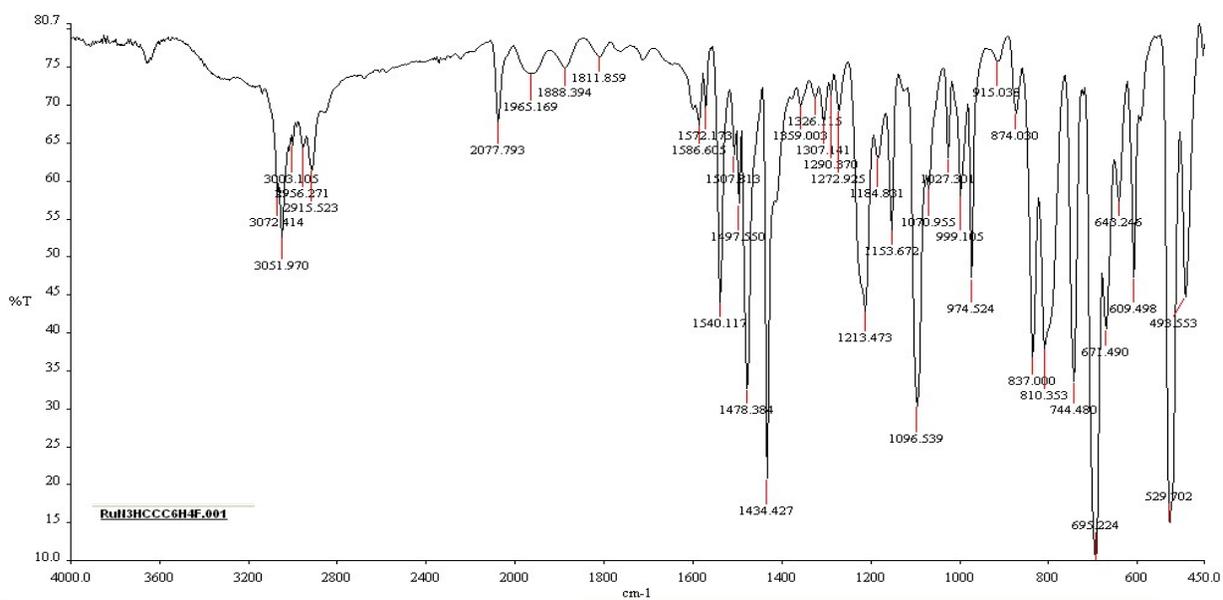
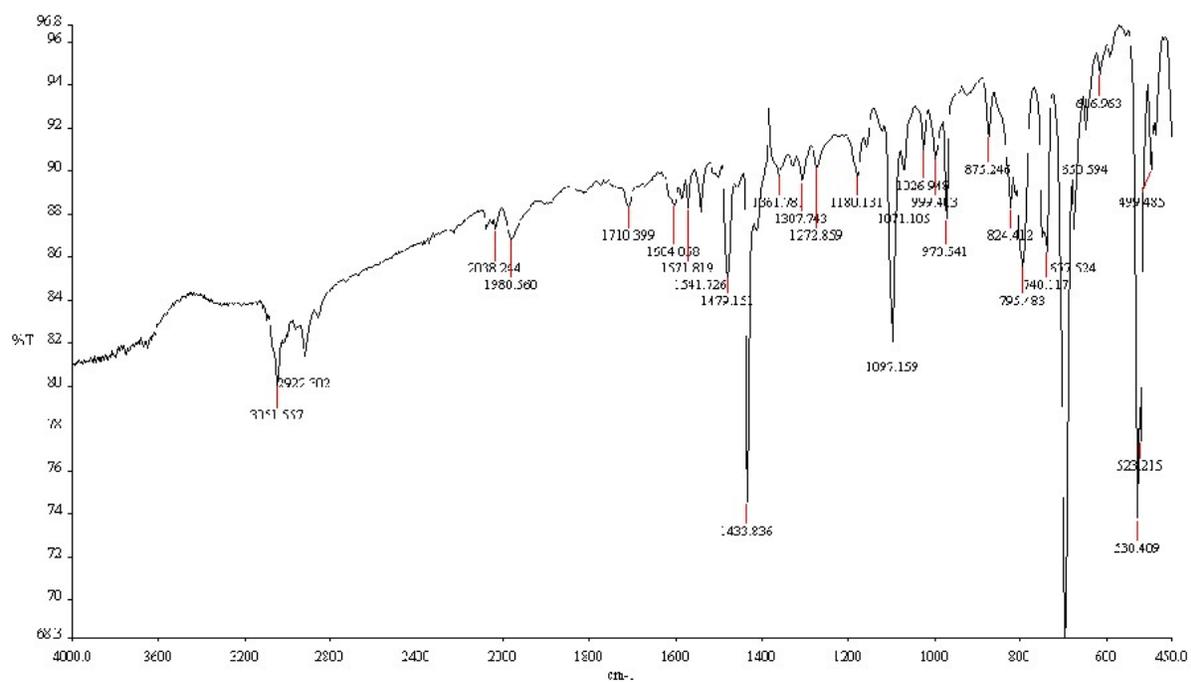


Fig. S12 IR spectra of compound 3,  $[\text{Ru}]\text{N}_3\text{C}_2\text{H}(4\text{-C}_6\text{H}_4\text{CHO})$ .





**Fig. S15** IR spectra of compound **6**, [Ru]N<sub>3</sub>C<sub>2</sub>H(4-C<sub>6</sub>H<sub>4</sub>CH<sub>3</sub>).