

## **Mercapto-benzothiazolyl based ruthenium(II) borate complexes: Synthesis and reactivity towards various phosphines**

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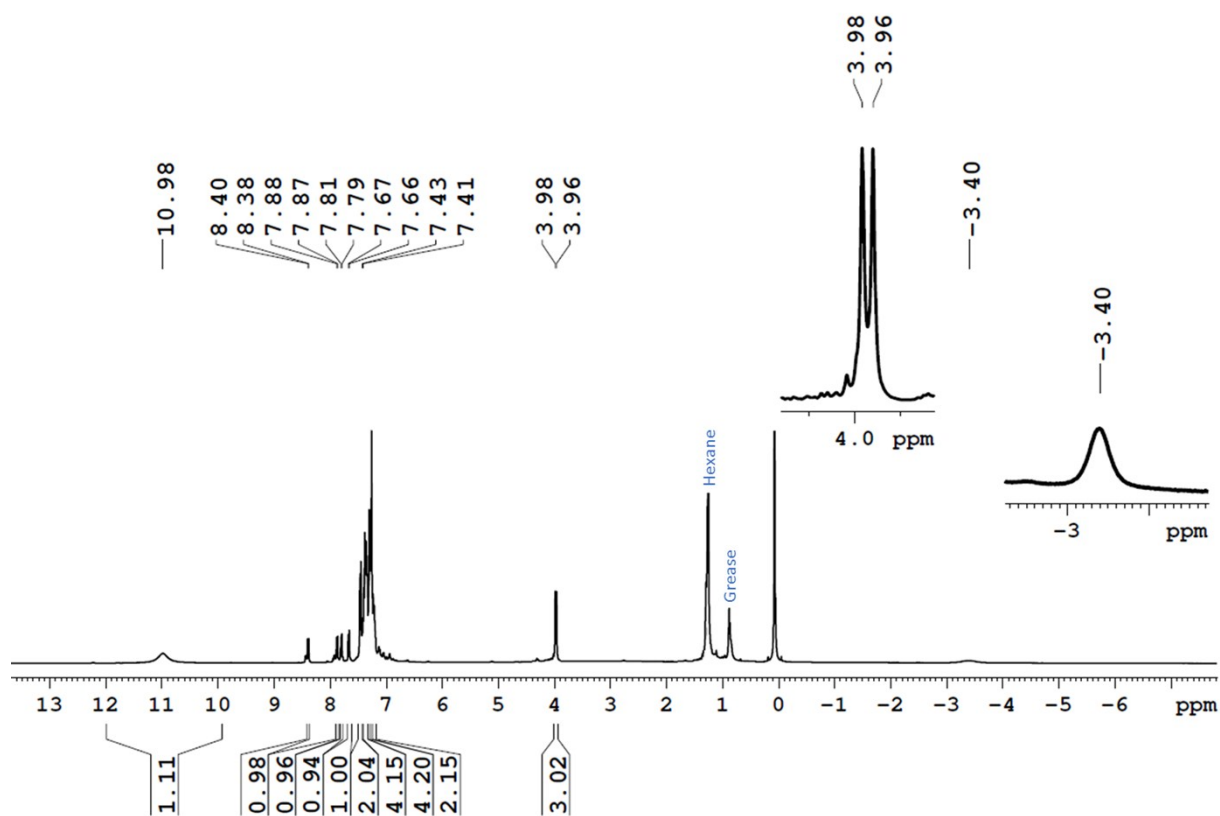
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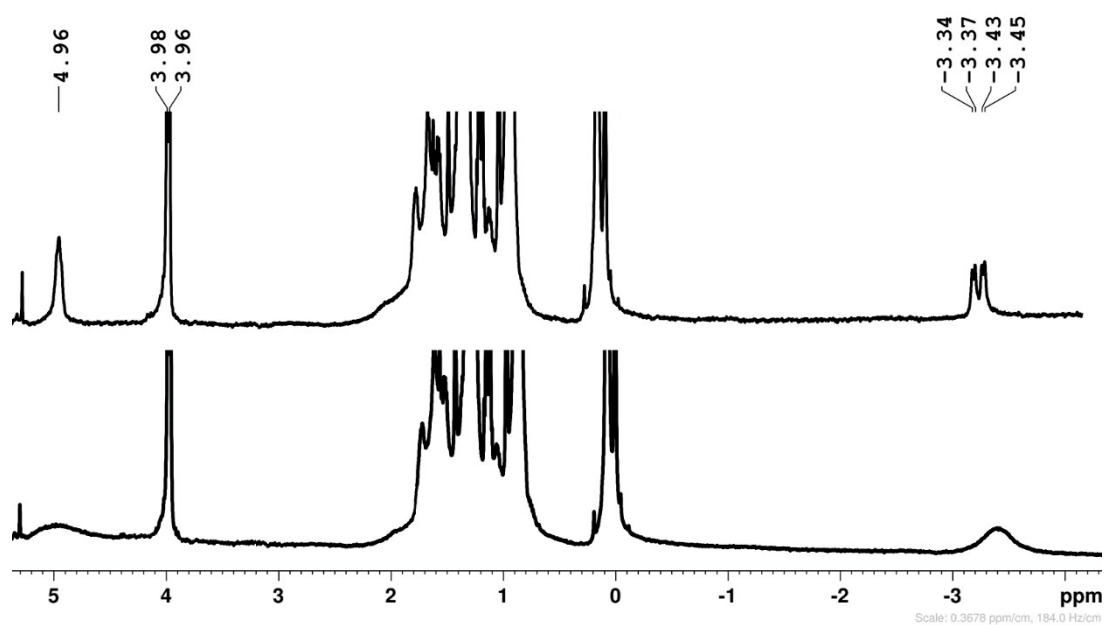
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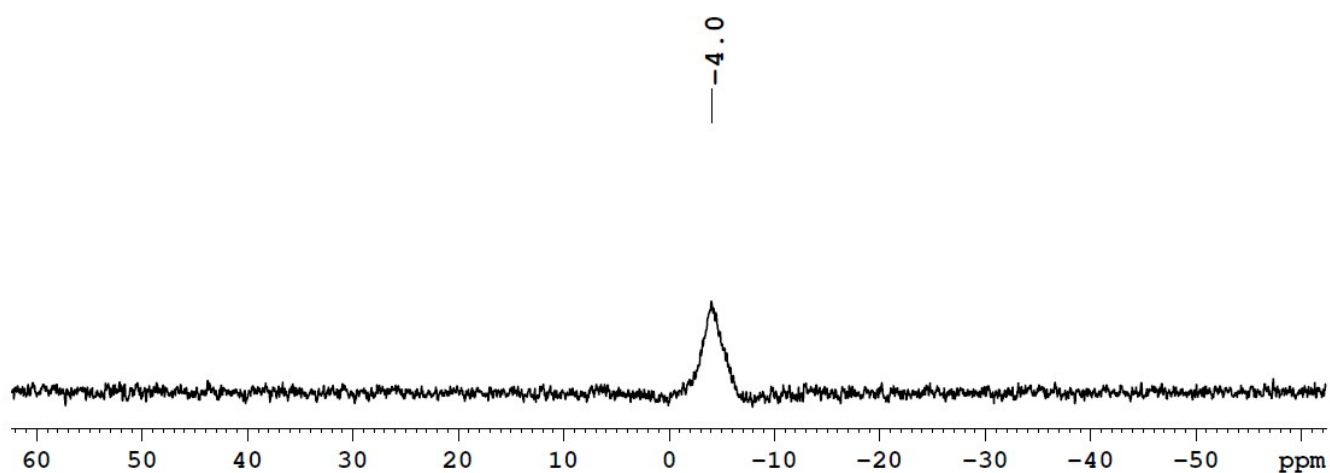
# I Spectroscopic details



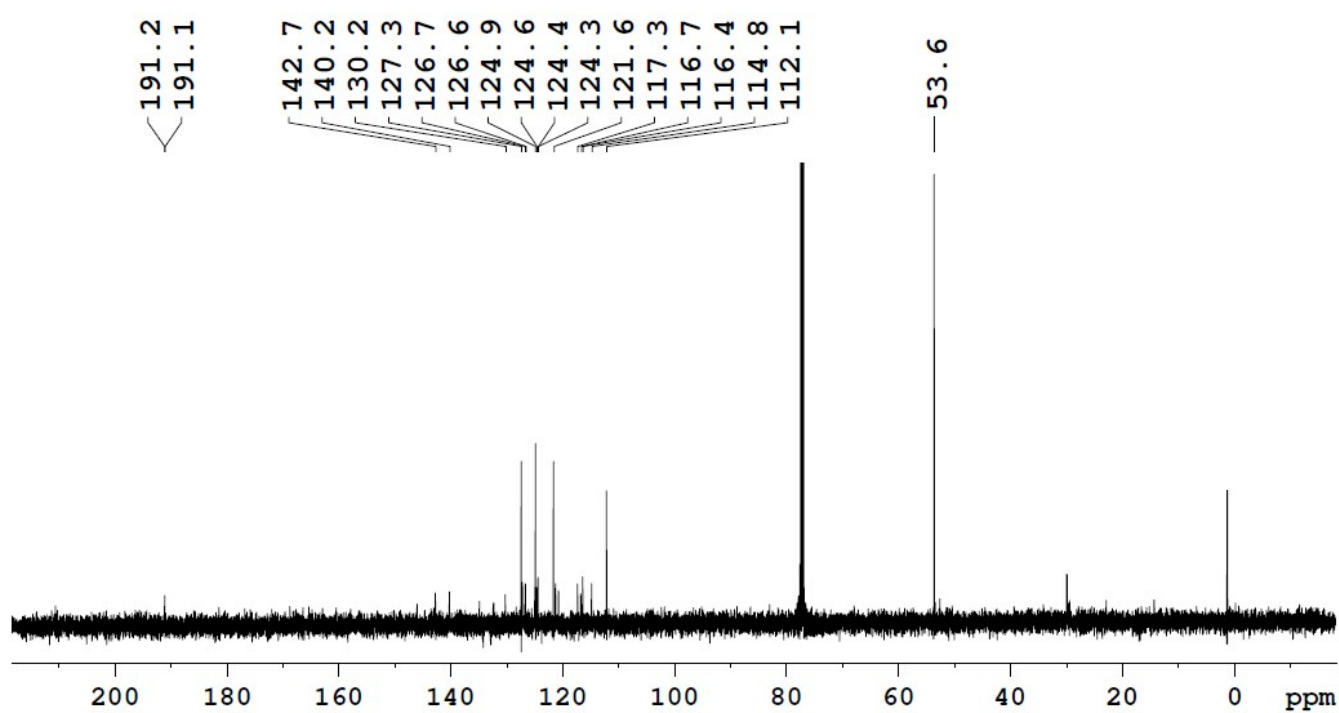
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**Fig. S2.** Stacked  $^1\text{H}$  (bottom) and  $^1\text{H}\{^{11}\text{B}\}$  NMR (top) spectrum of **2**.



**Fig. S3.**  $^{11}\text{B}\{^1\text{H}\}$  NMR spectrum of **2**.



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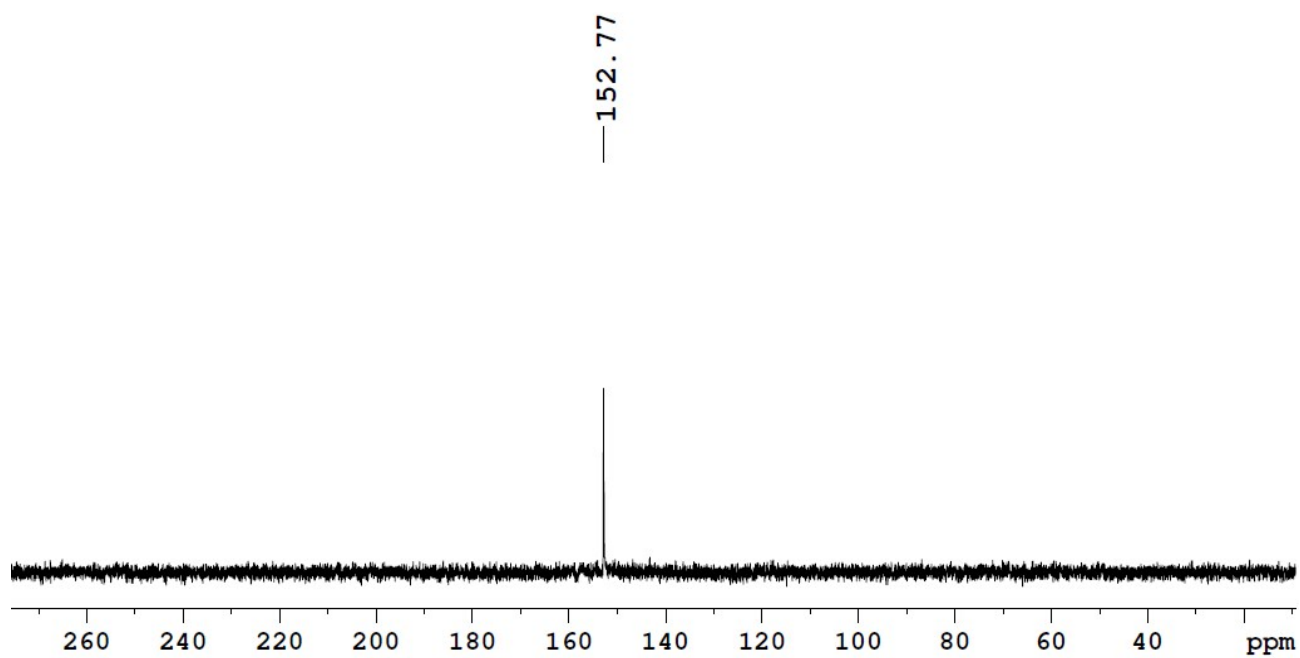


Fig. S5.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **2**.

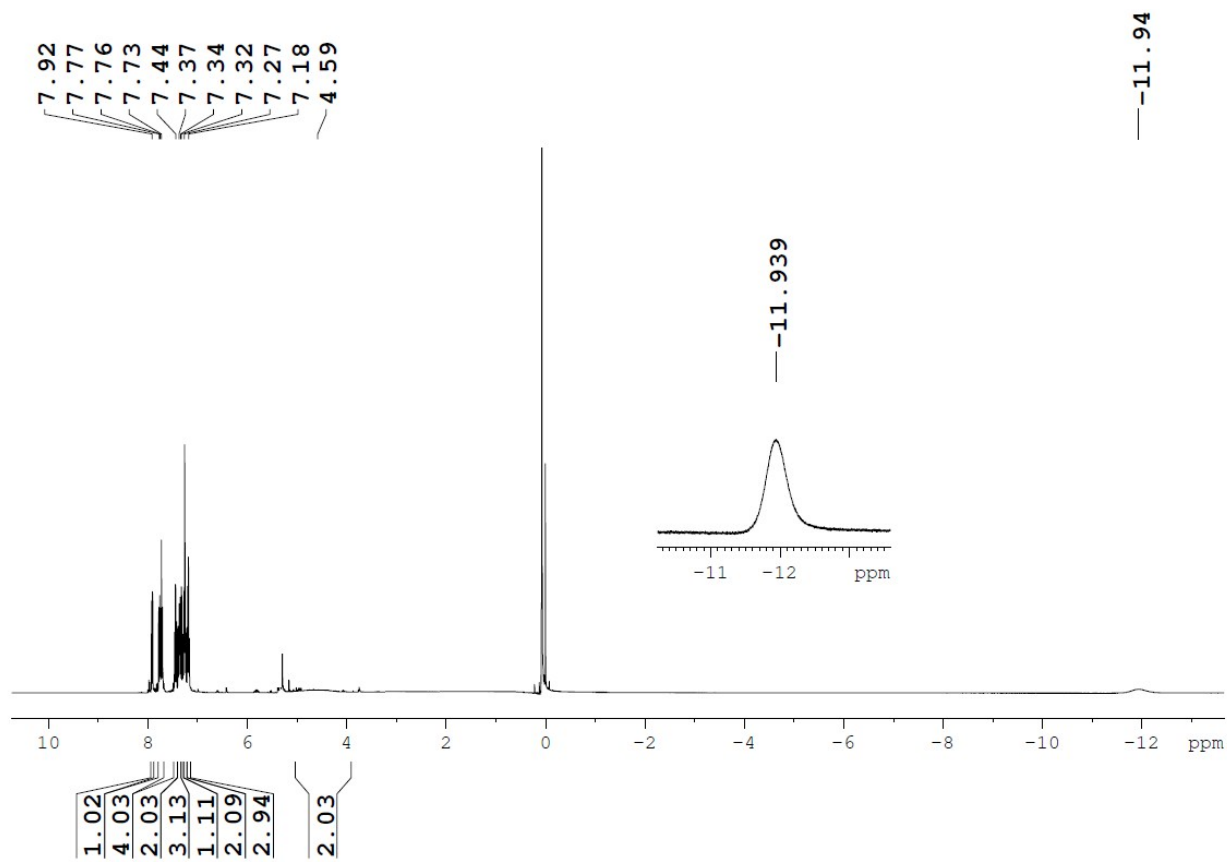
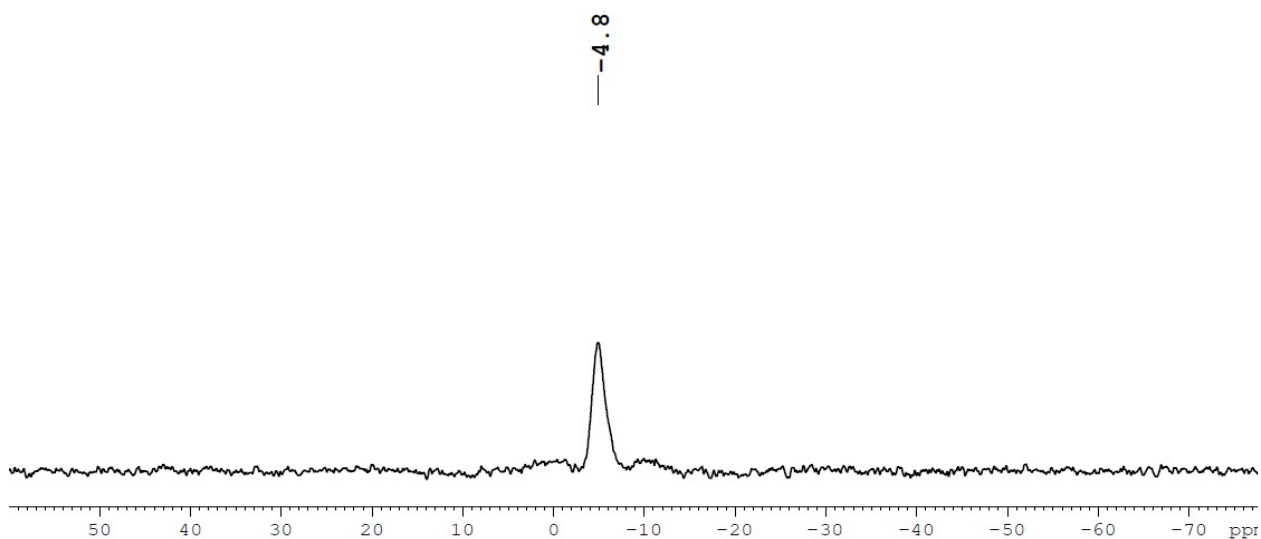
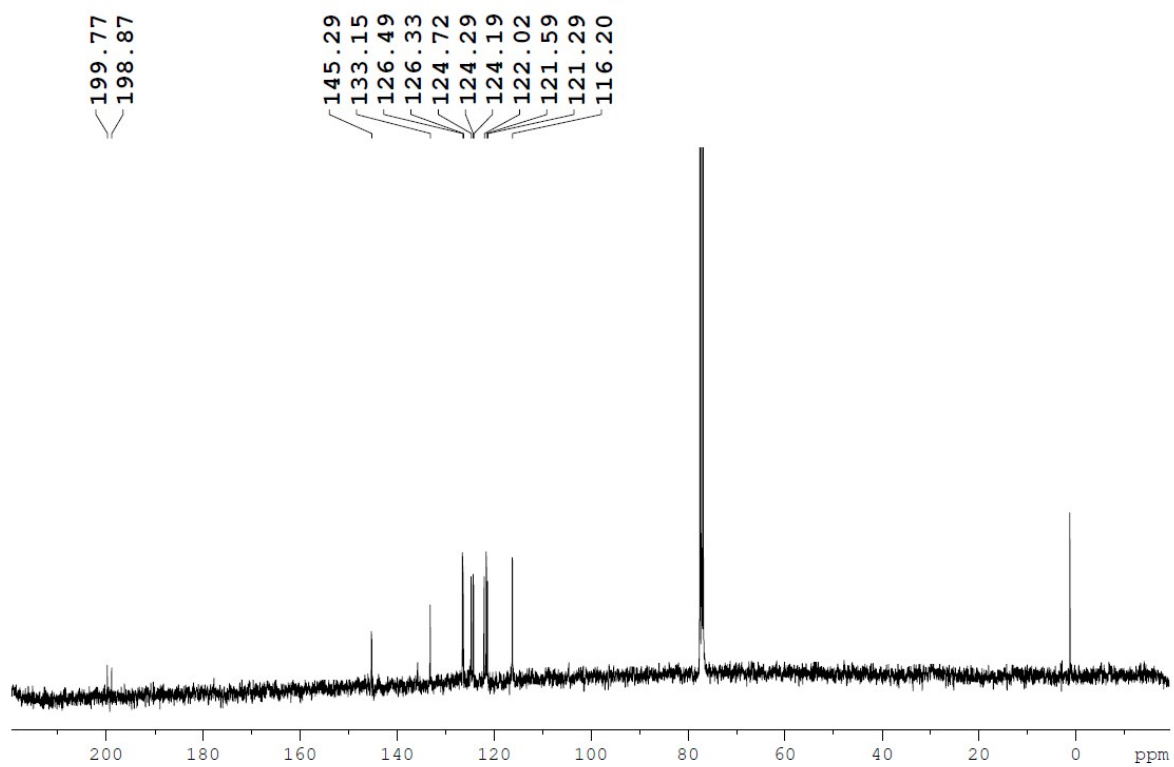


Fig. S6.  $^1\text{H}$  NMR spectrum of **3**.



**Fig. S7.**  $^{11}\text{B}\{^1\text{H}\}$  NMR spectrum of **3**.



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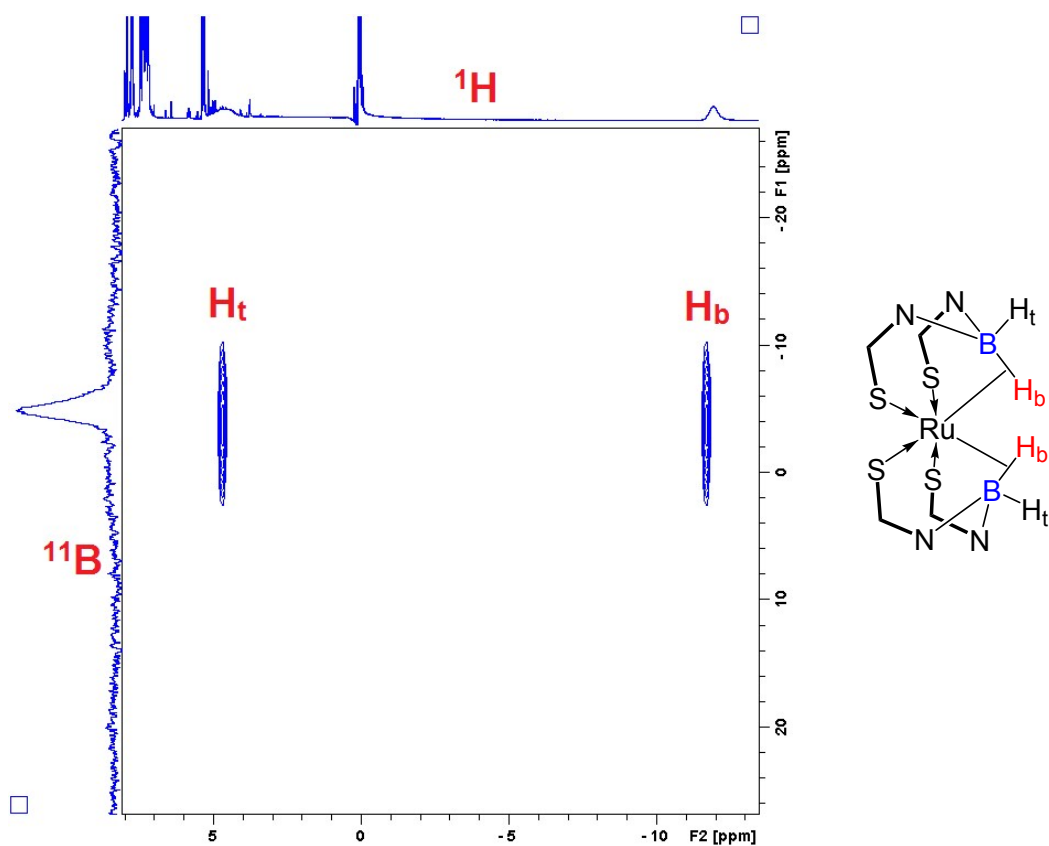


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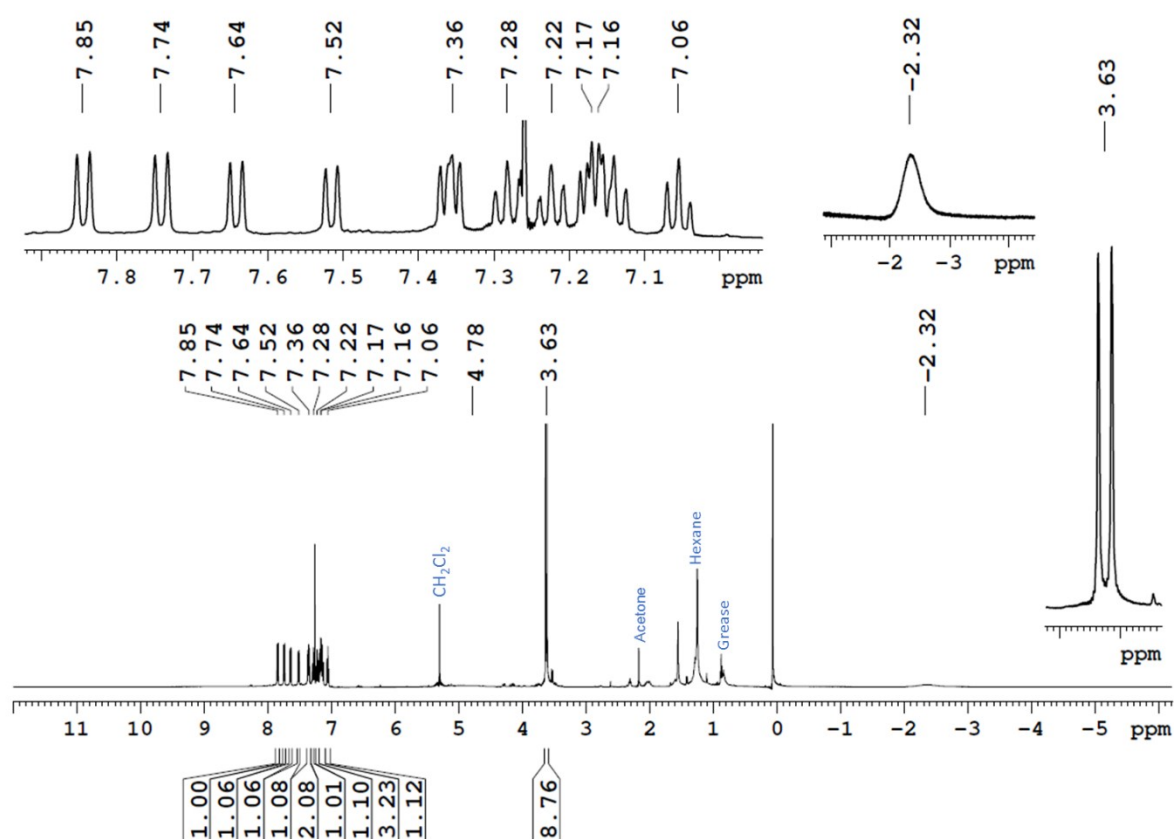
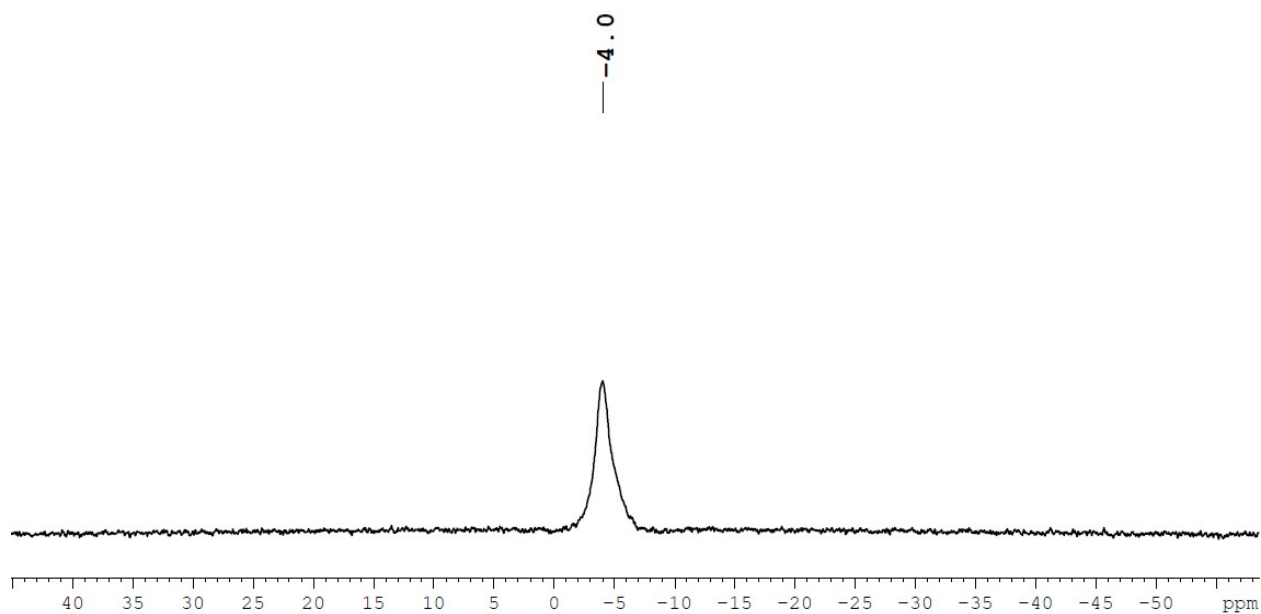
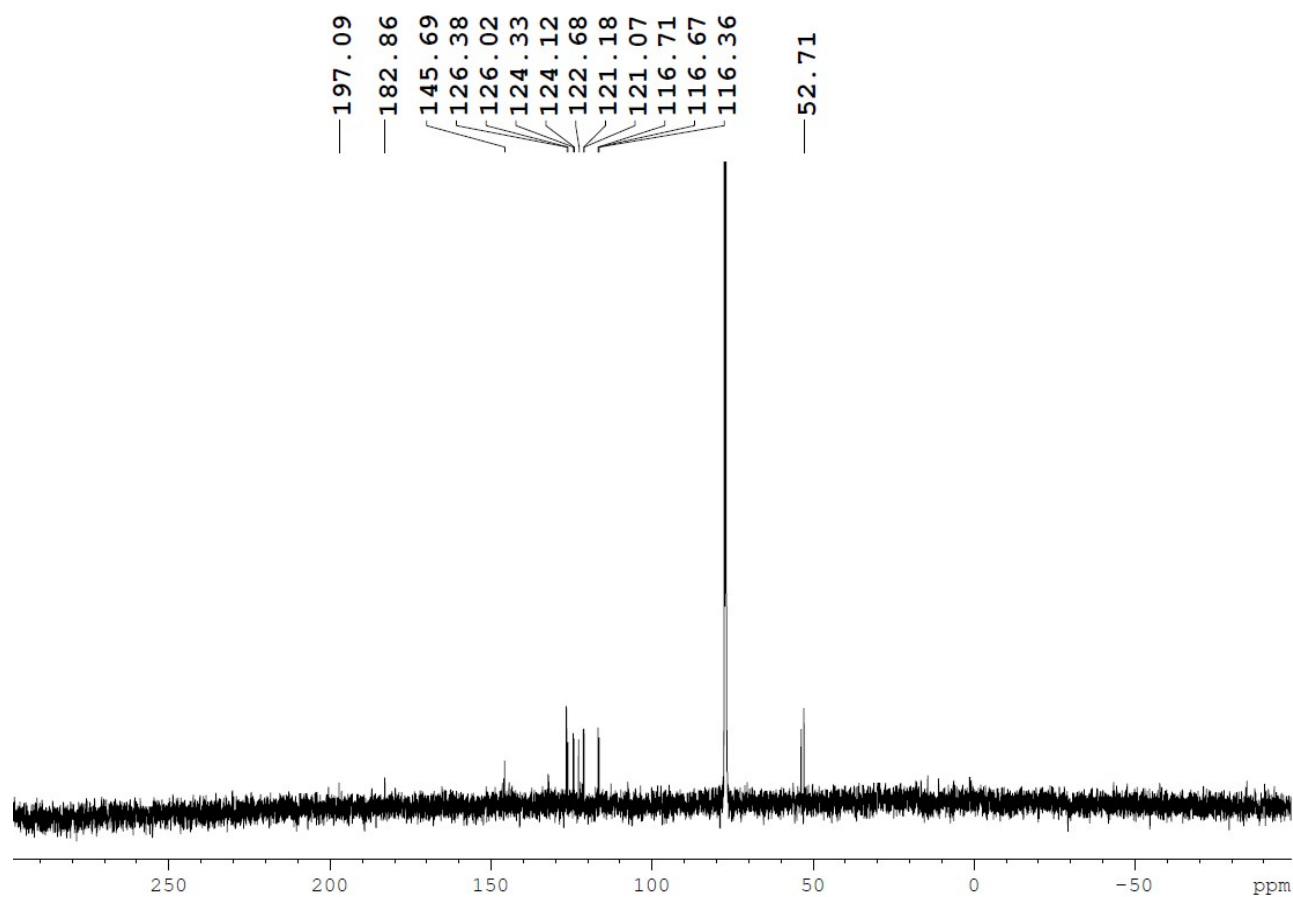


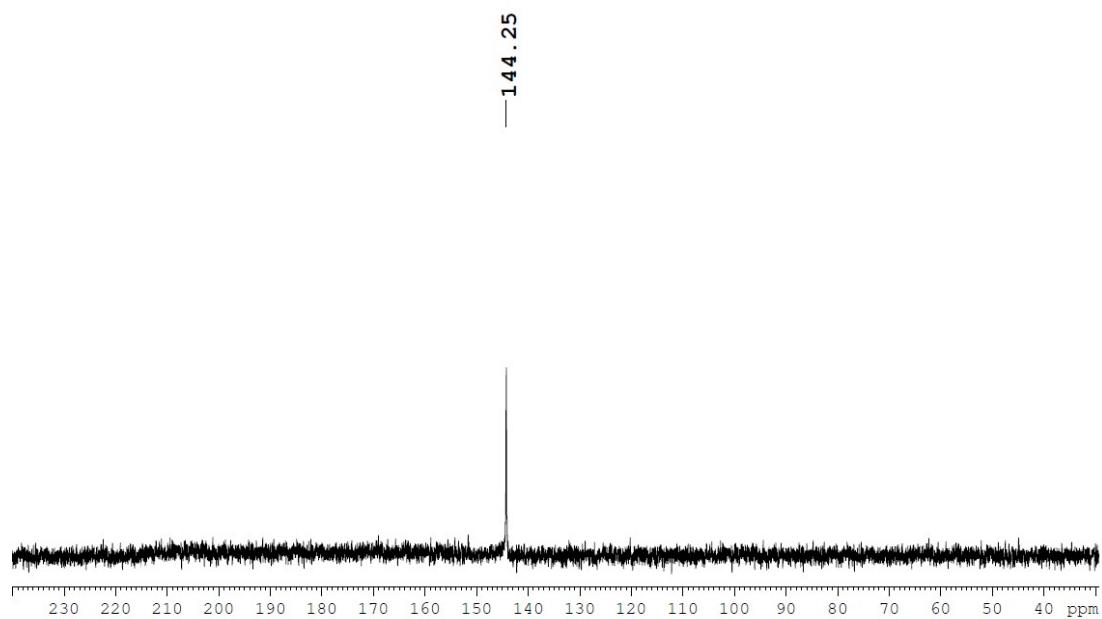
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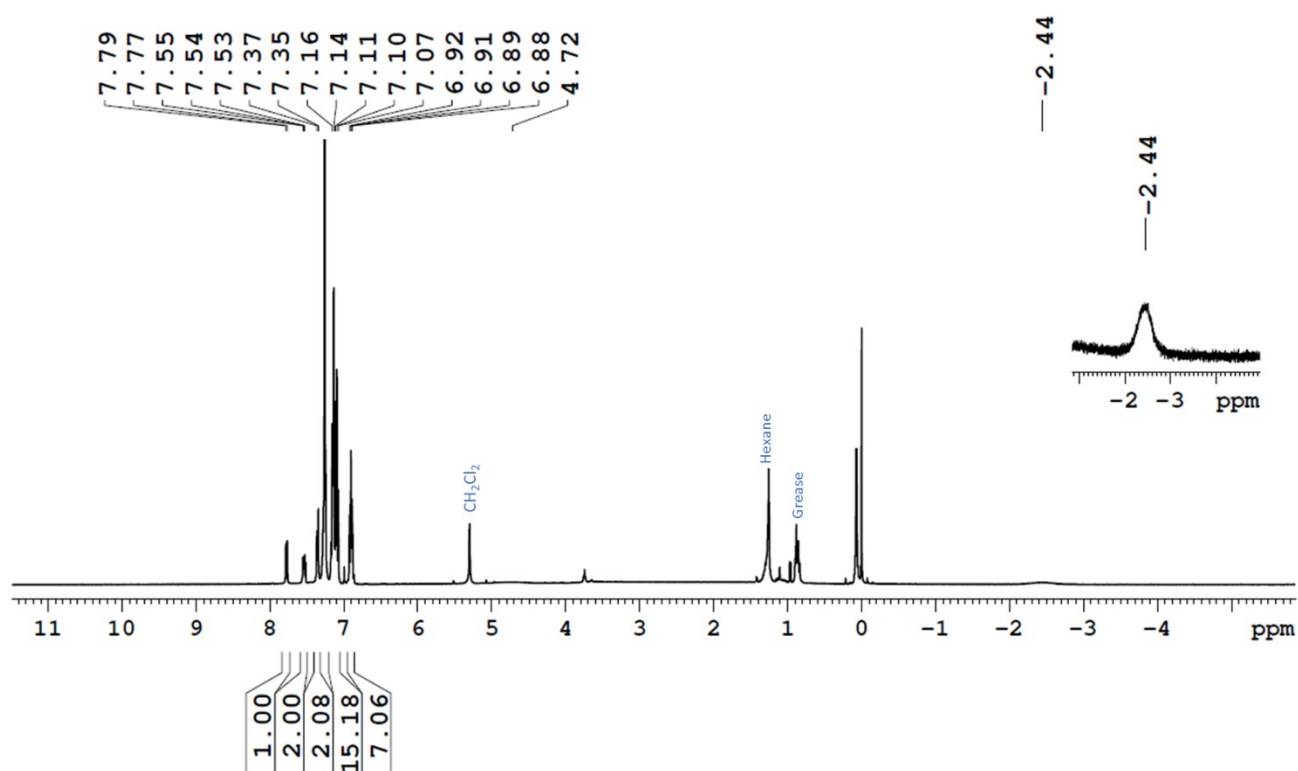
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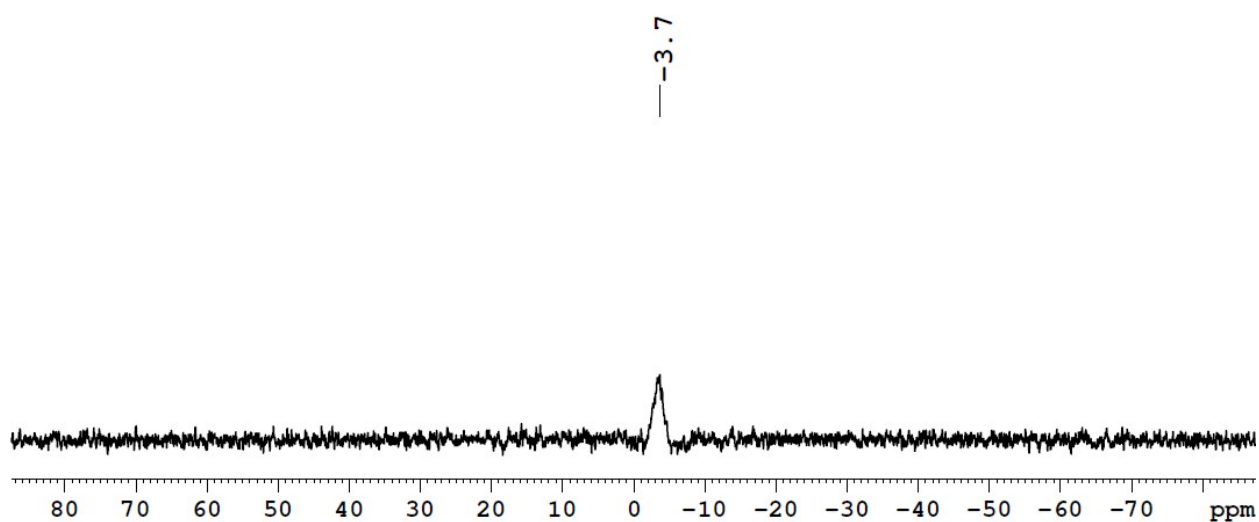


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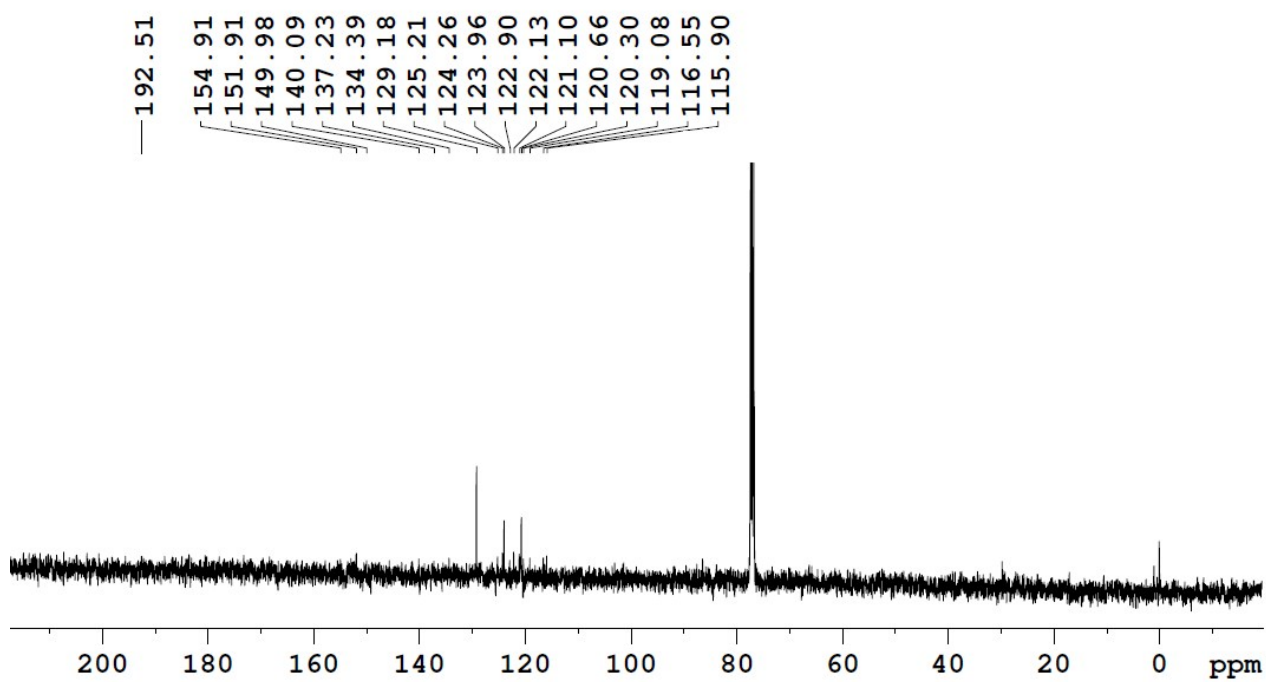


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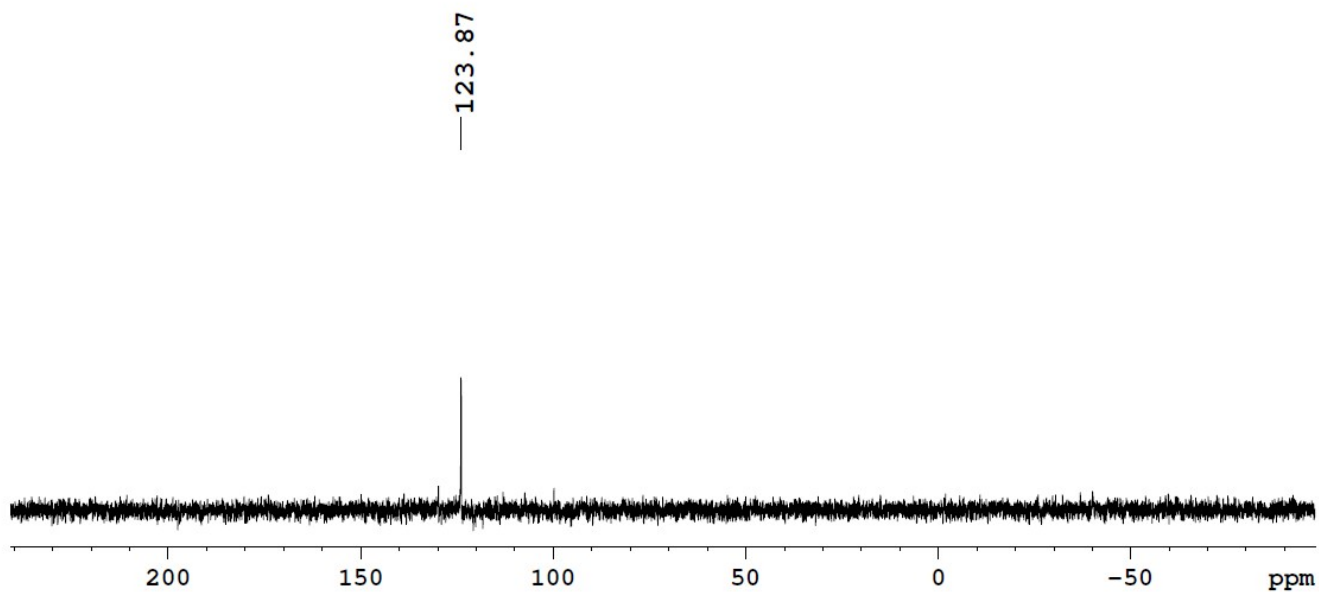


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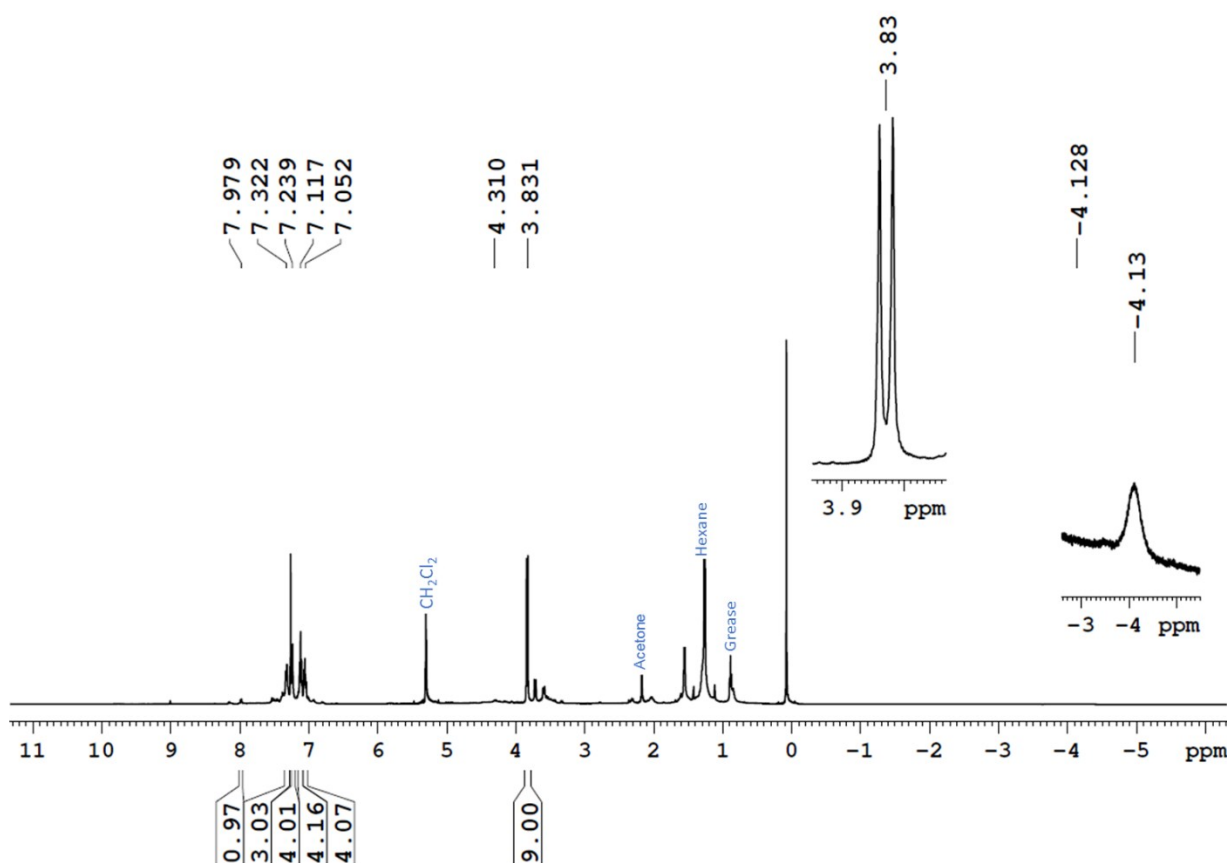


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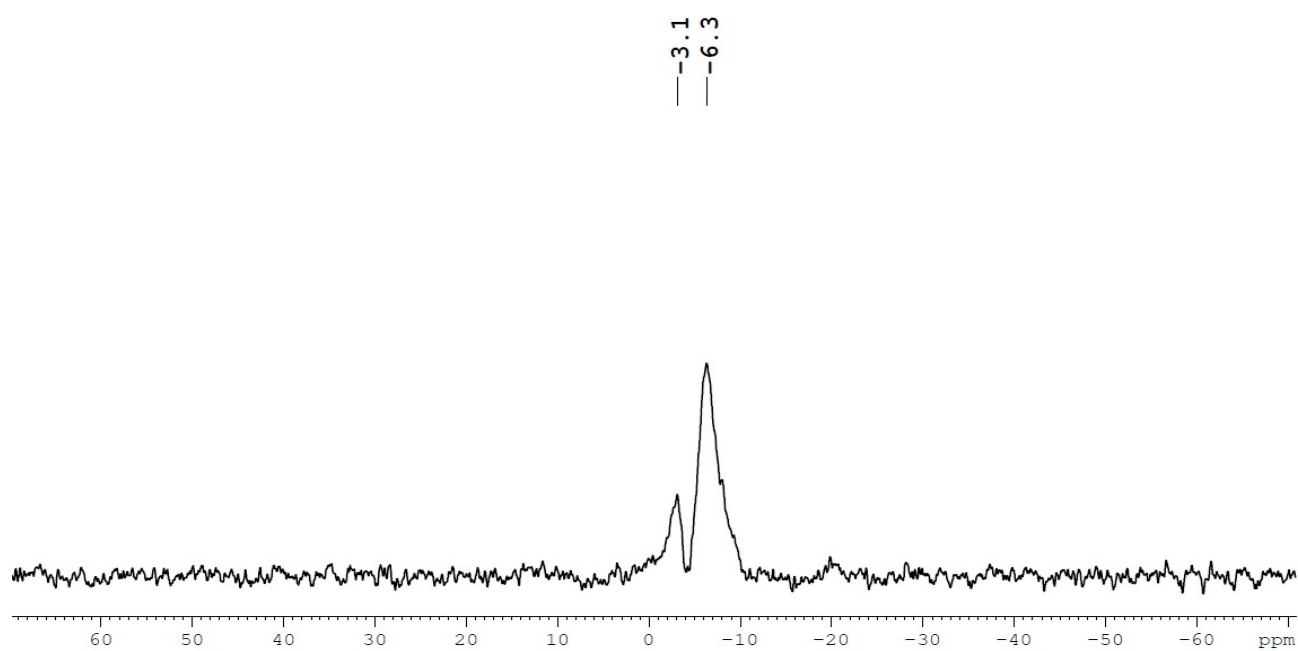


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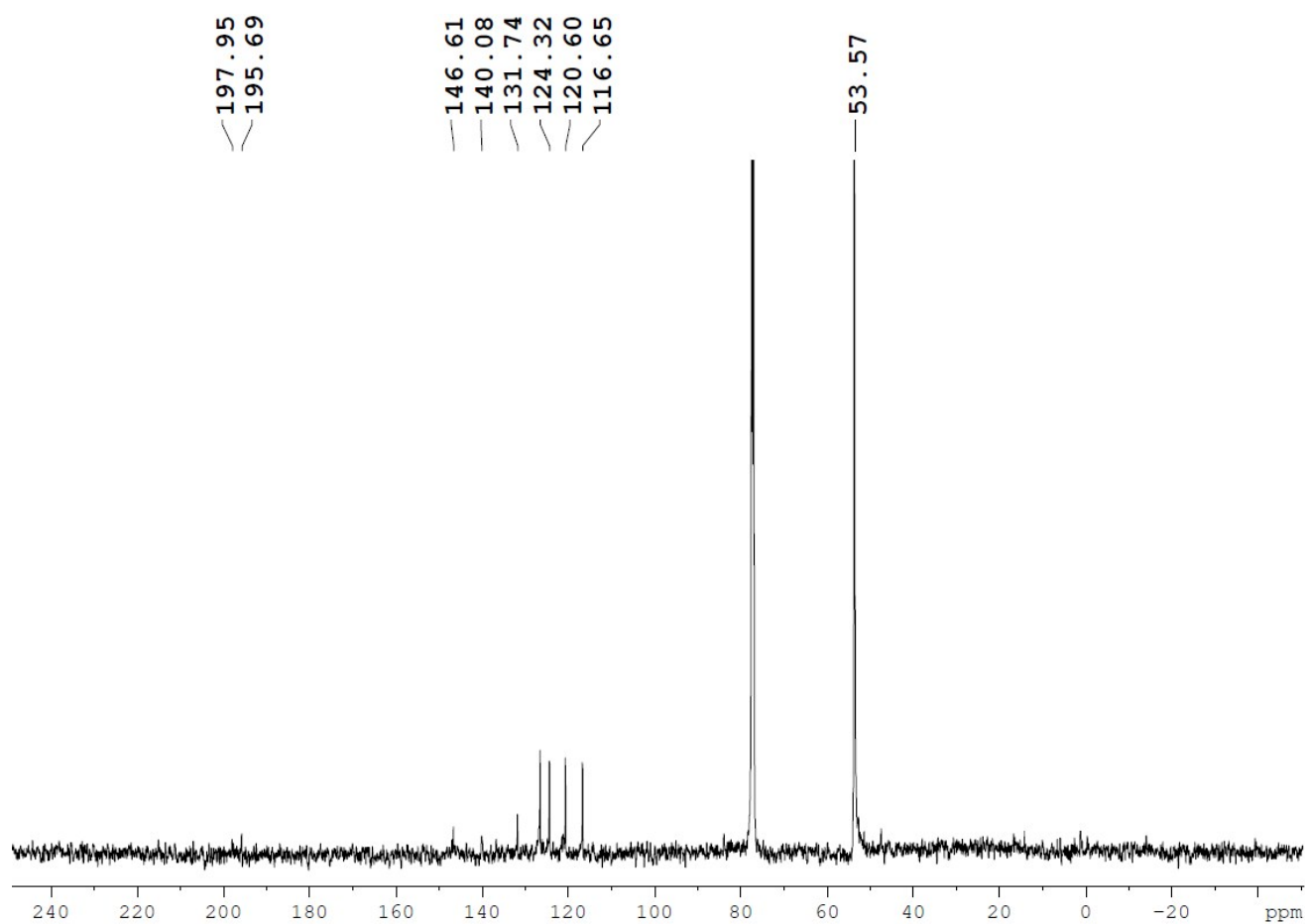


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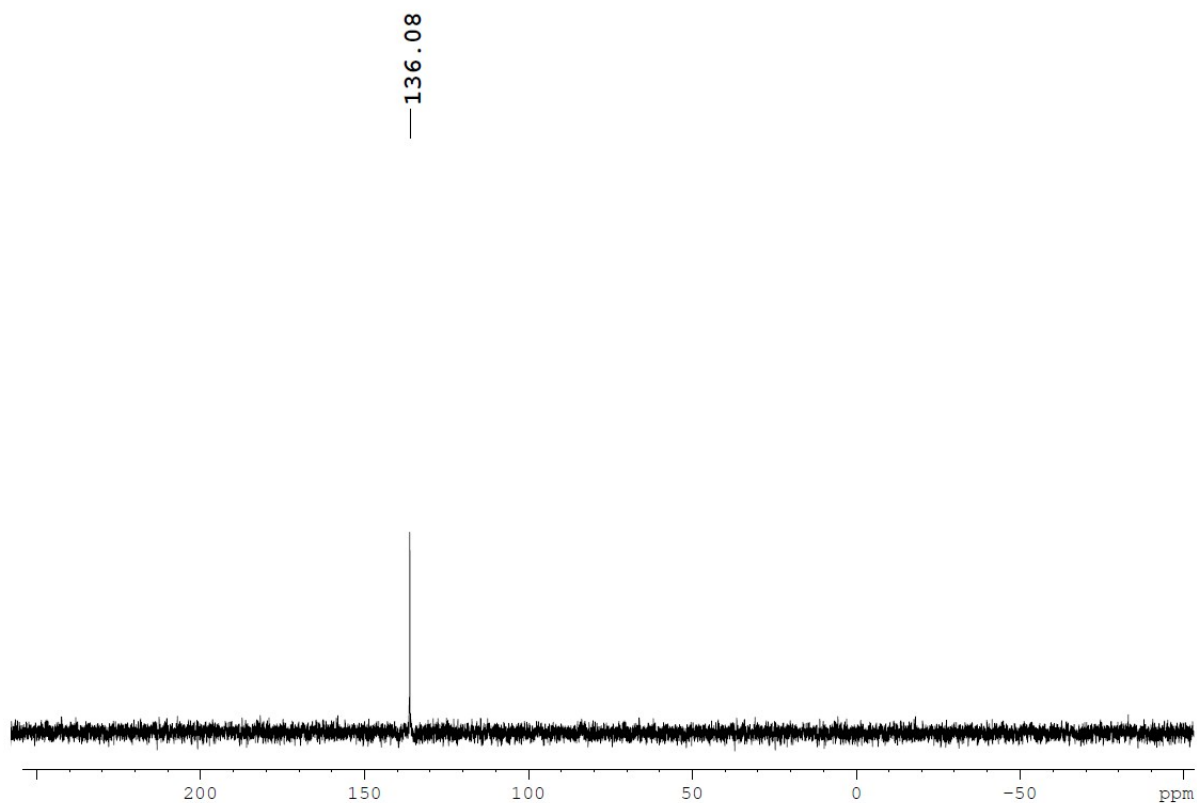


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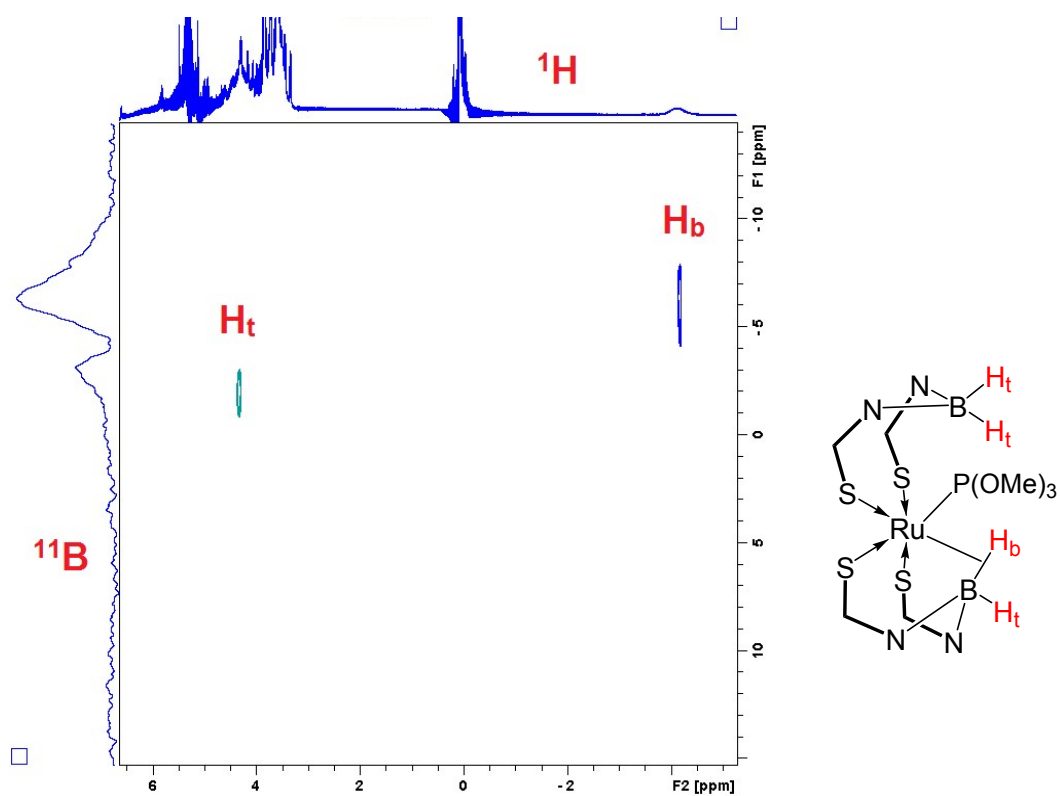


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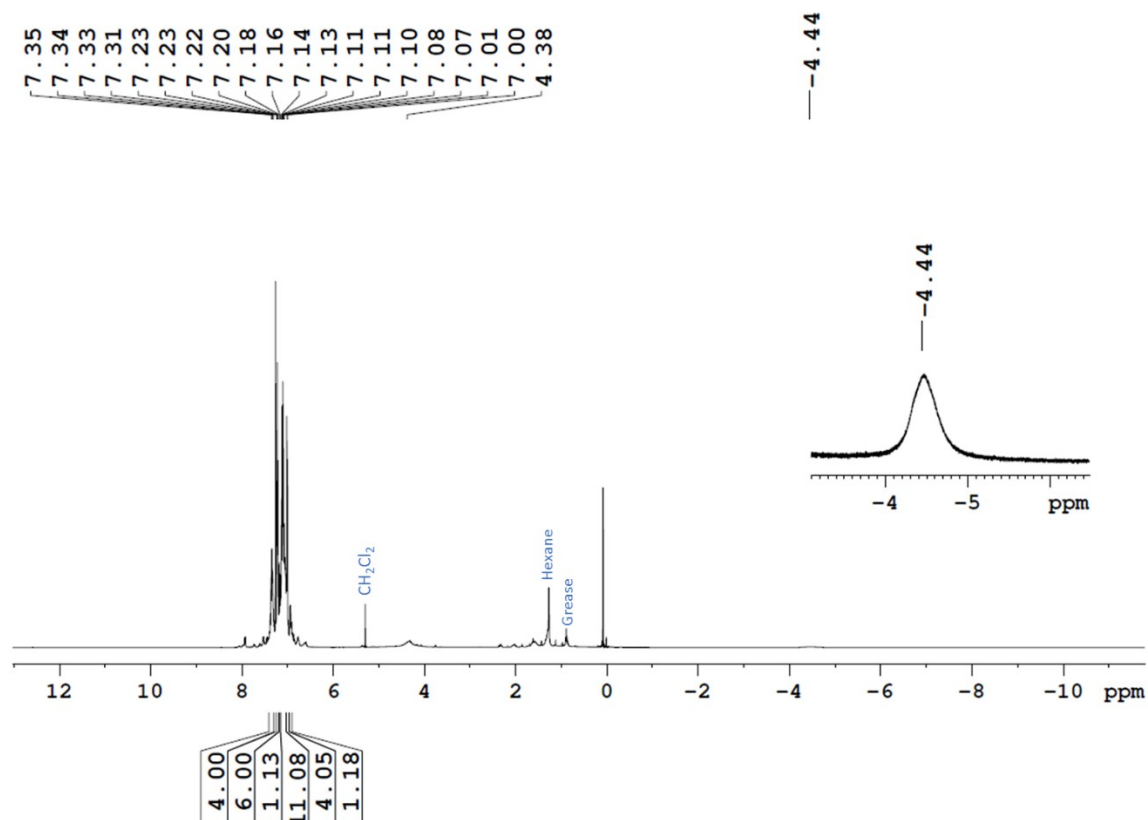


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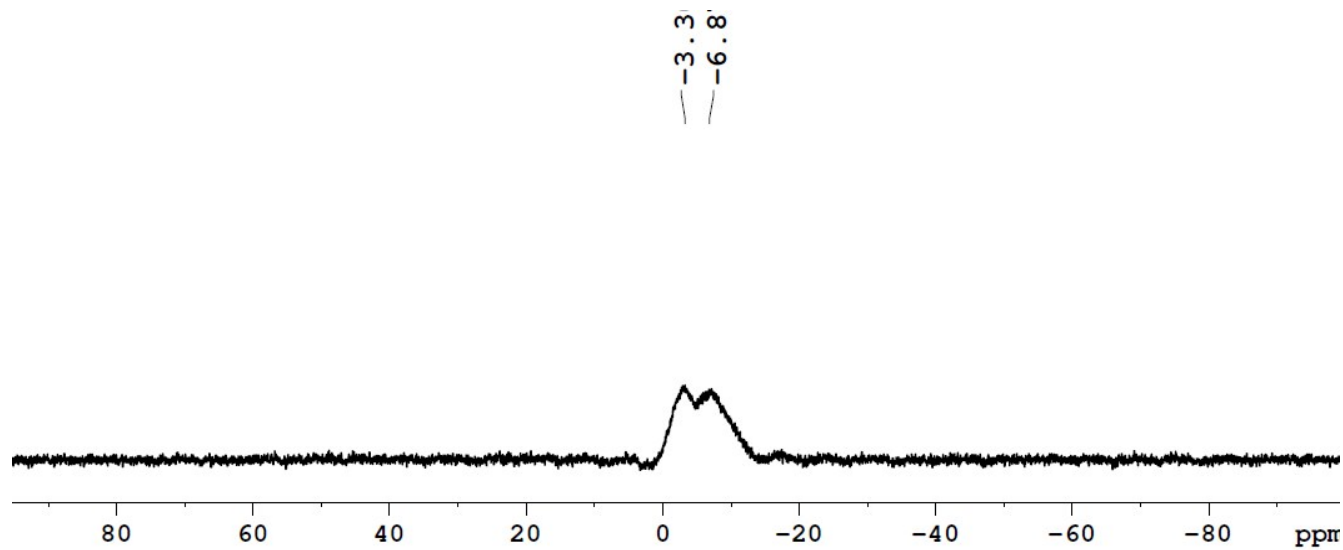


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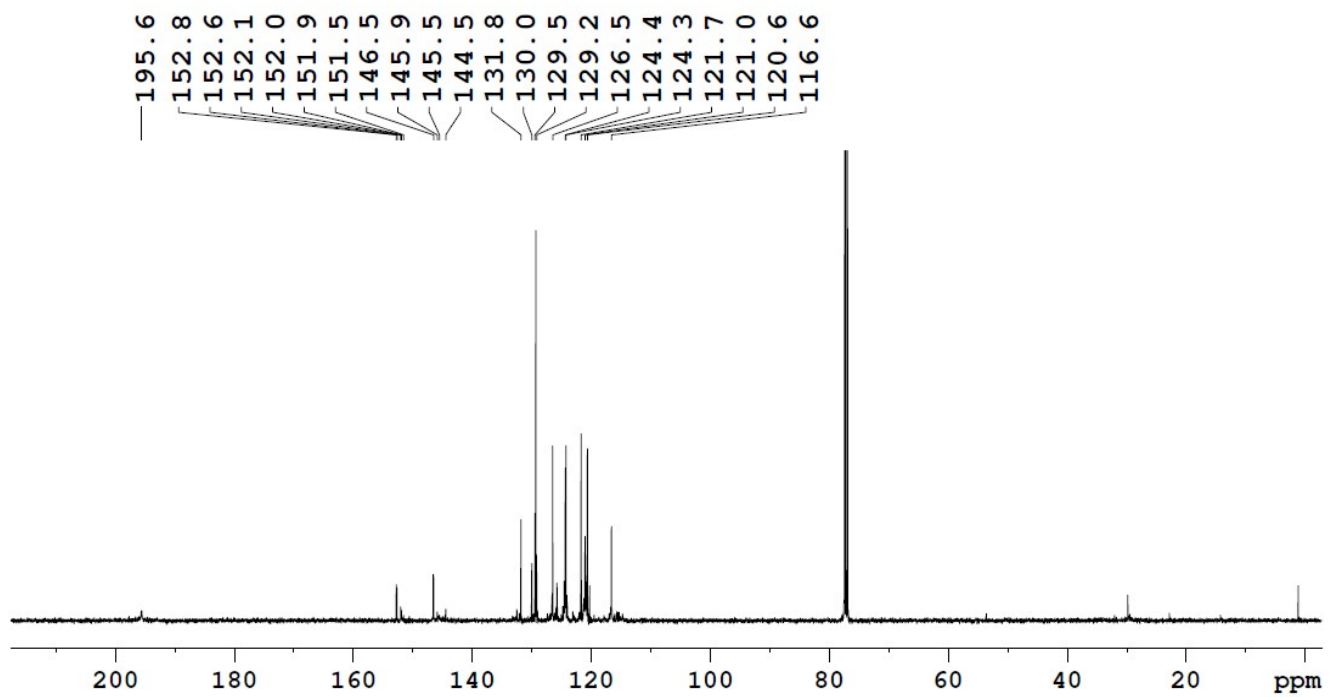


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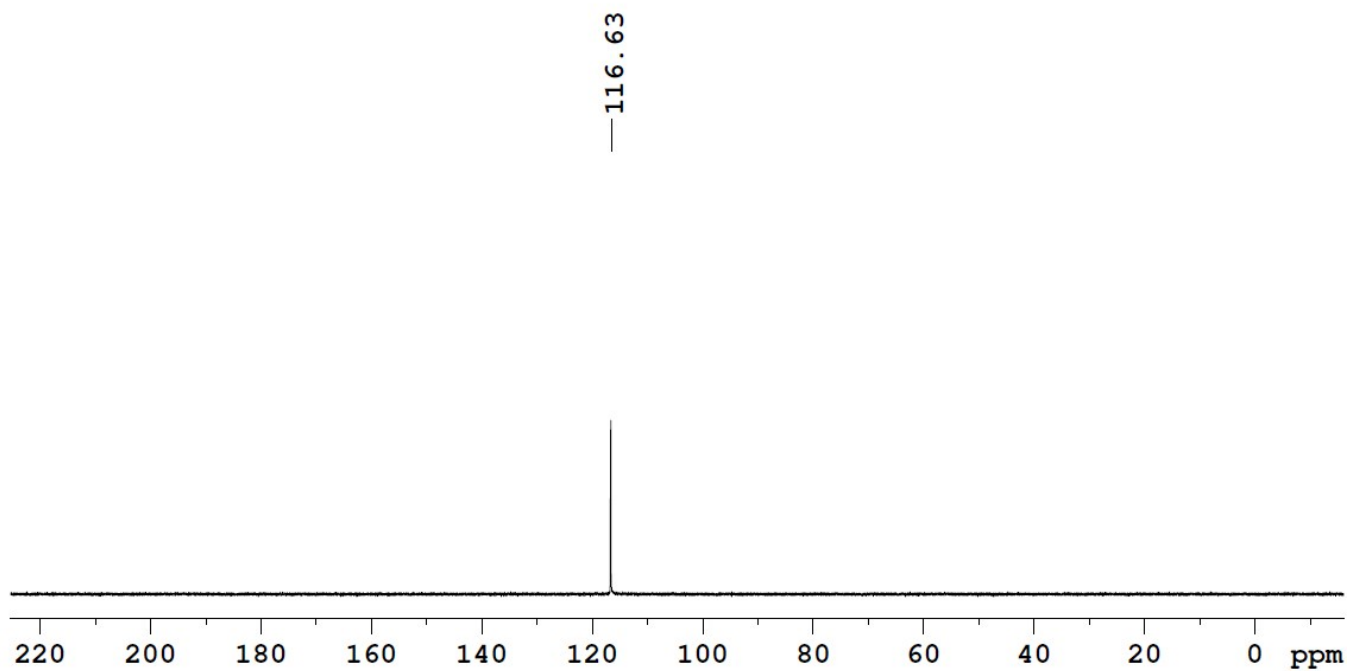


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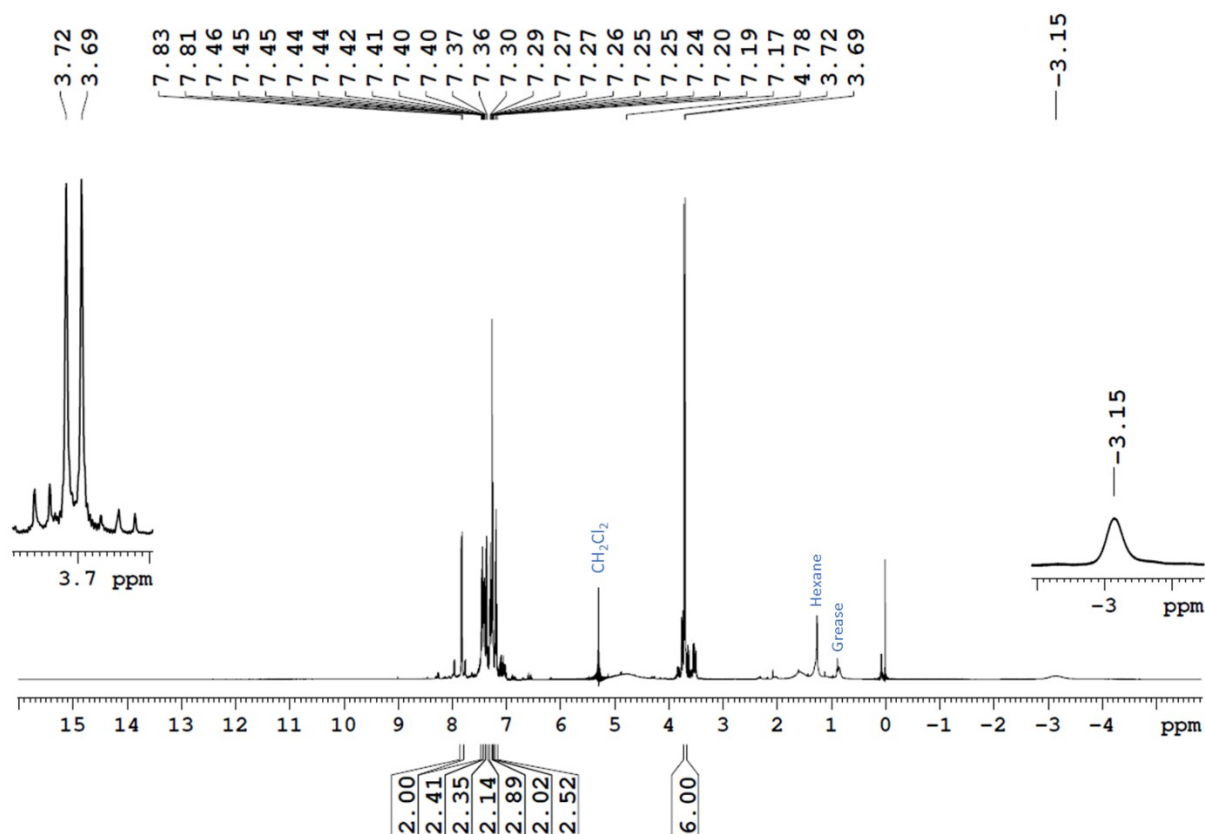


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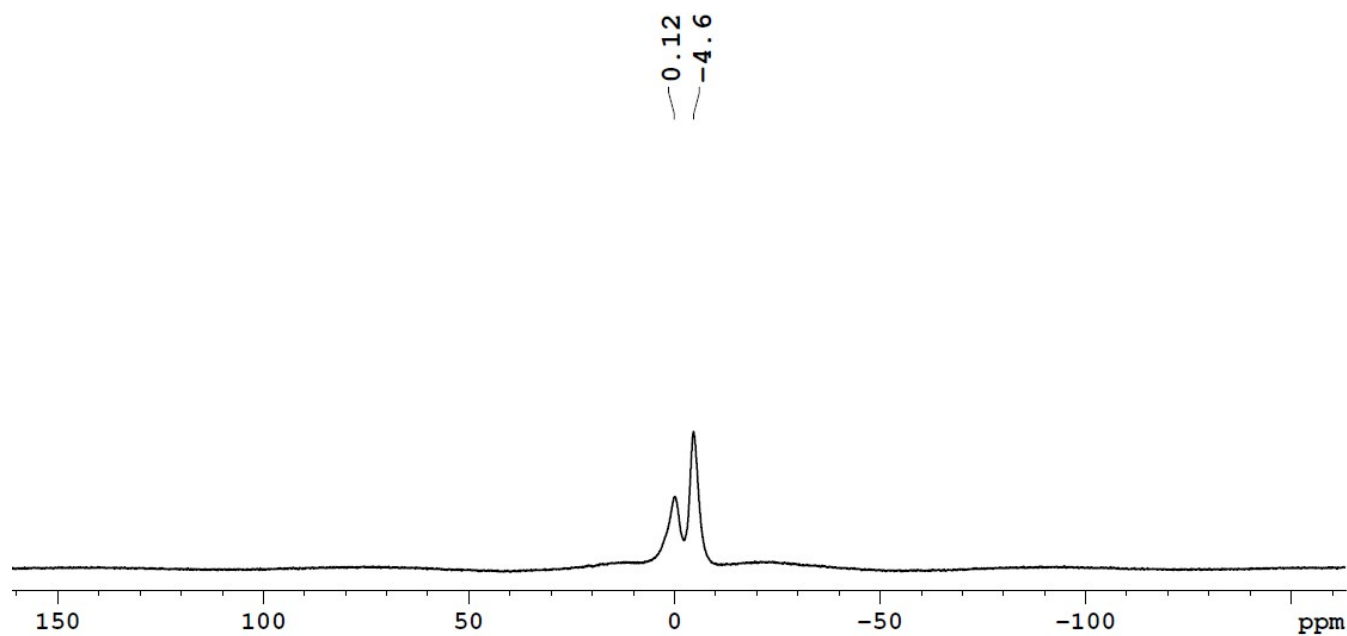


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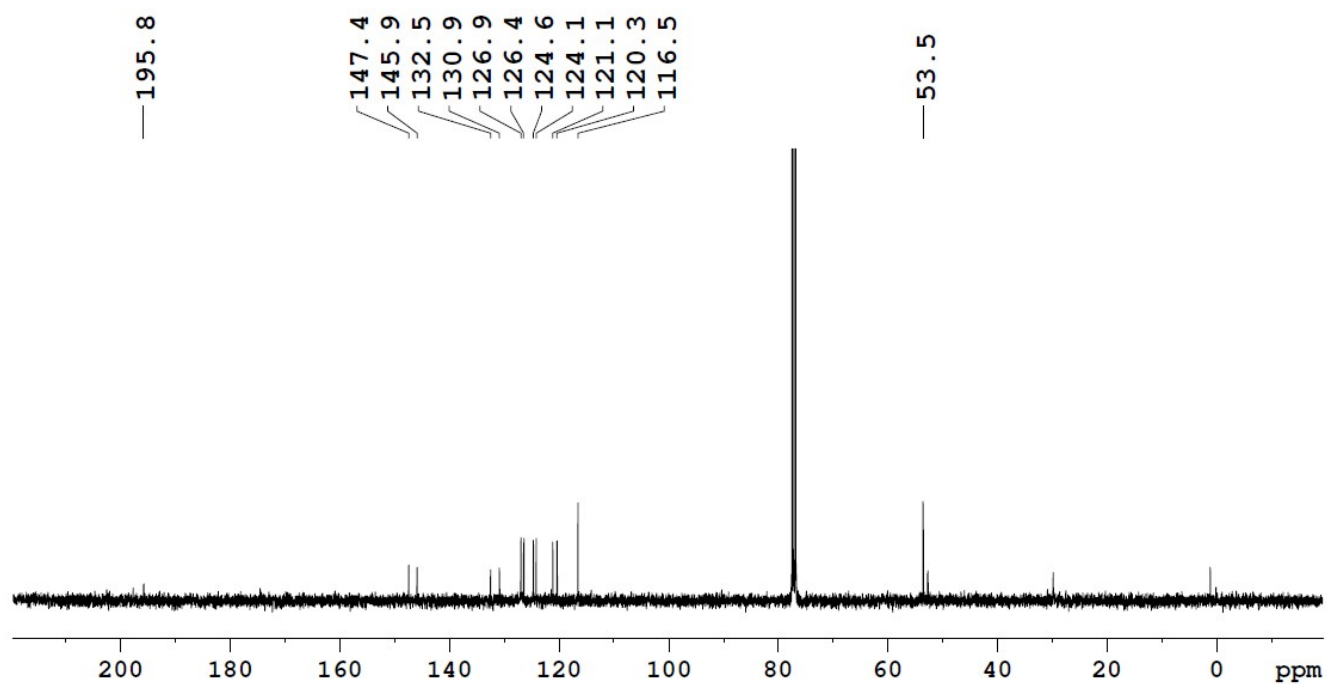


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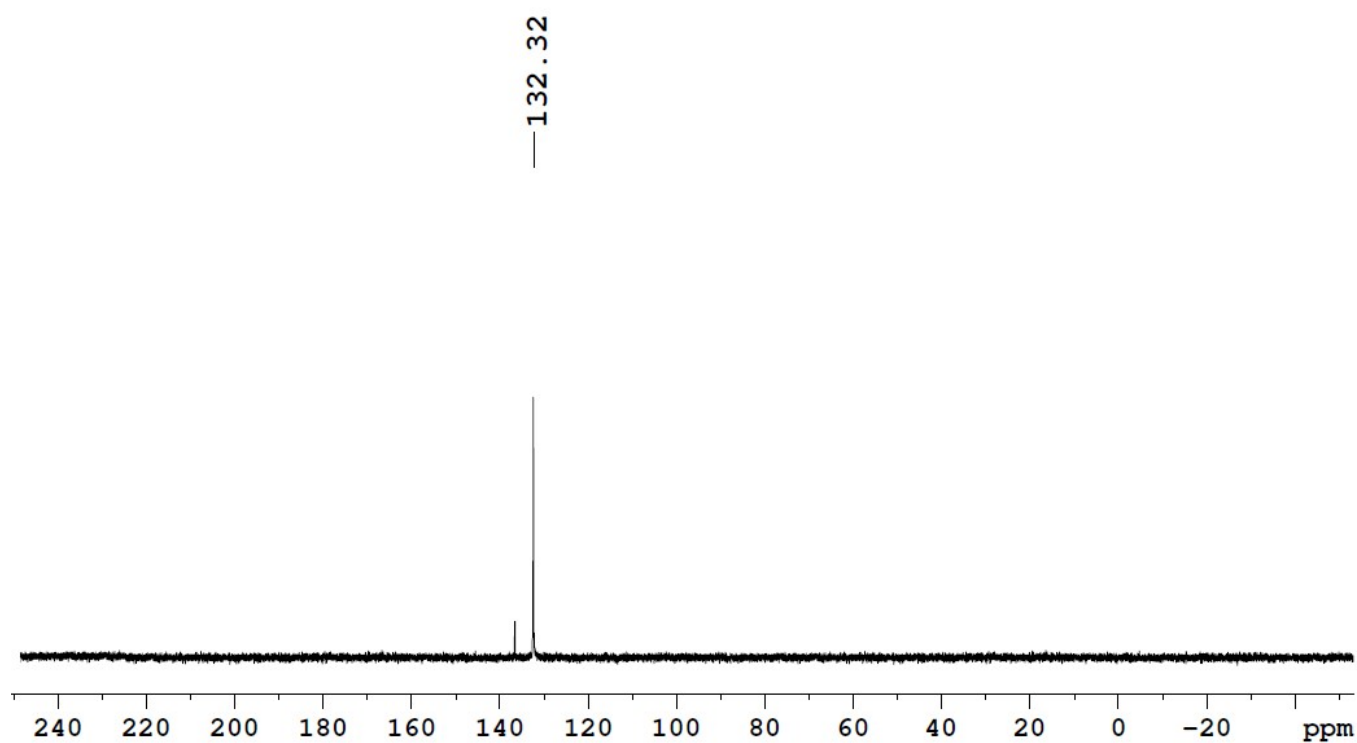
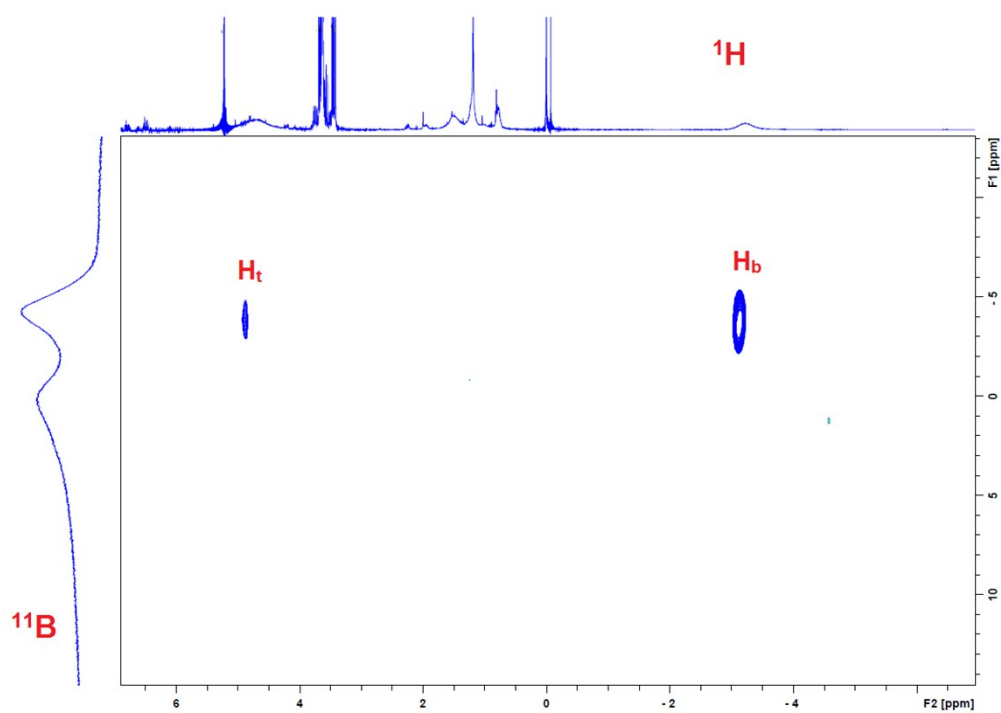
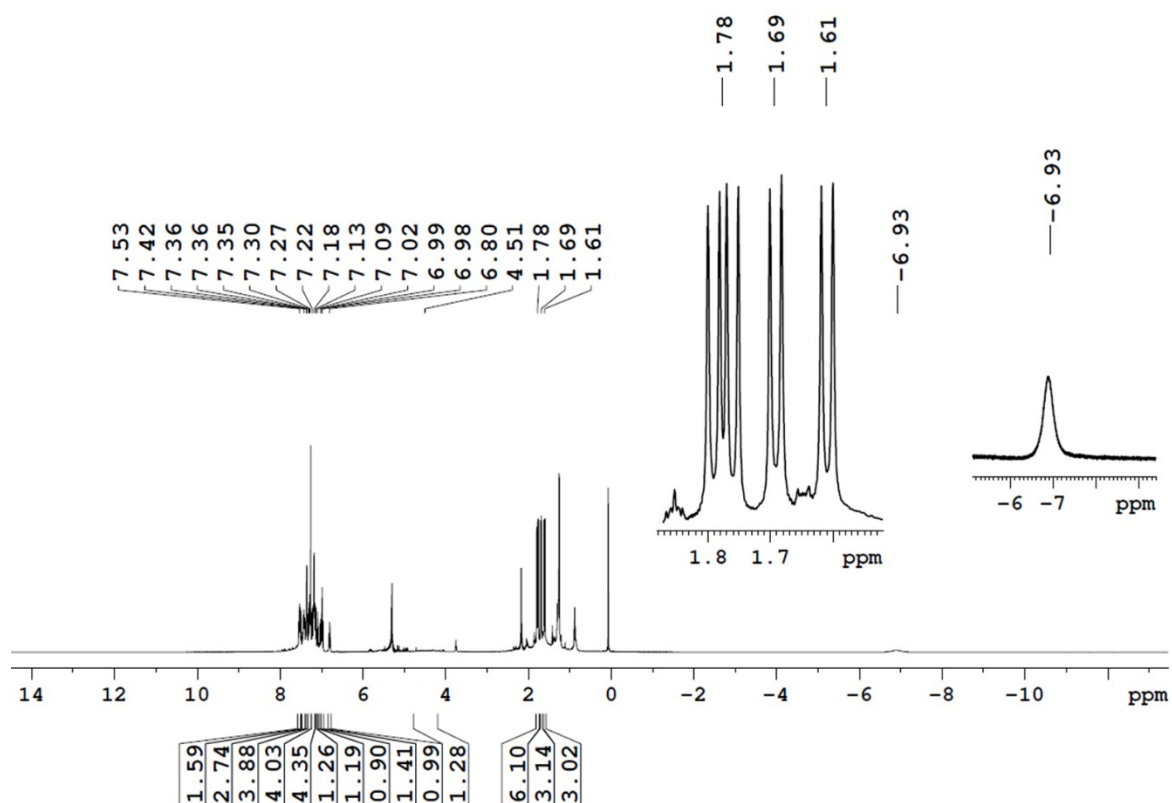


Fig. S30.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **6a**.

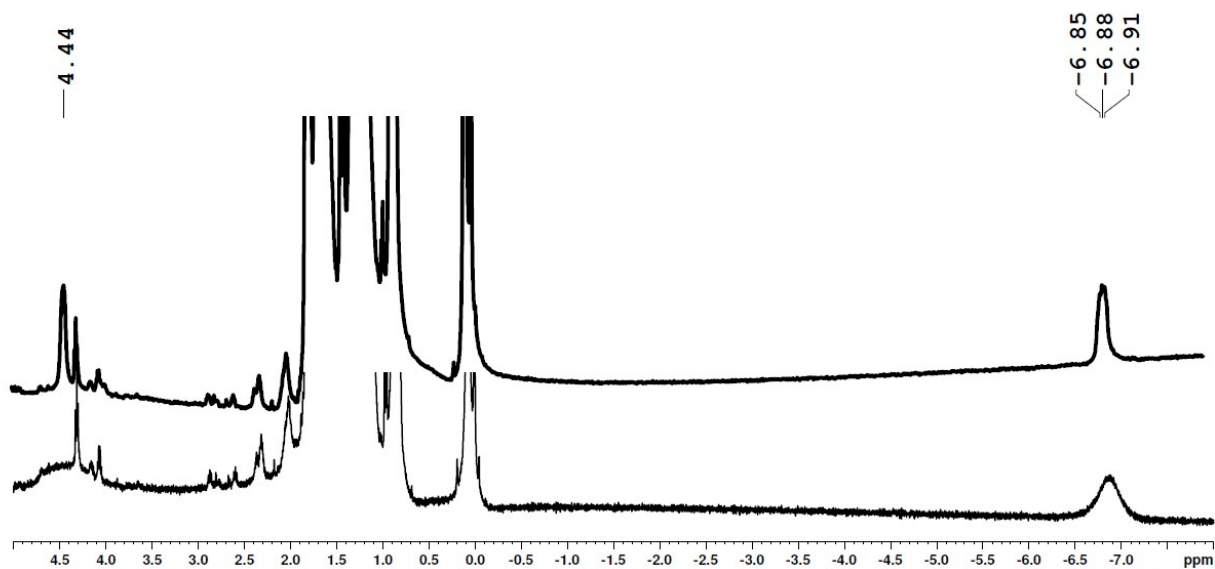




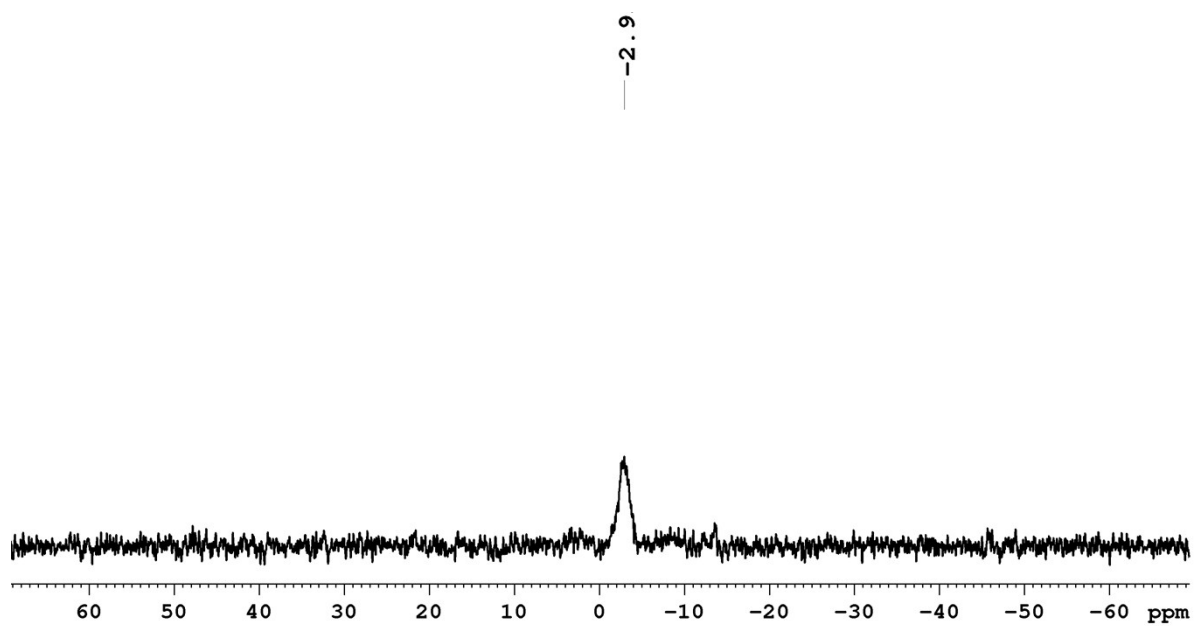
**Fig. S31.**  $^1\text{H}\{^{11}\text{B}\}/^{11}\text{B}\{^1\text{H}\}$  HSQC spectrum of **6a**.



**Fig. S32.**  $^1\text{H}$  NMR spectrum of **7a**.



**Fig. S33.** Stacked  $^1\text{H}$  (bottom) and  $^1\text{H}\{^{11}\text{B}\}$  NMR (top) spectrum of **7a**.



**Fig. S34.**  $^{11}\text{B}\{^1\text{H}\}$  NMR spectrum of **7a**.

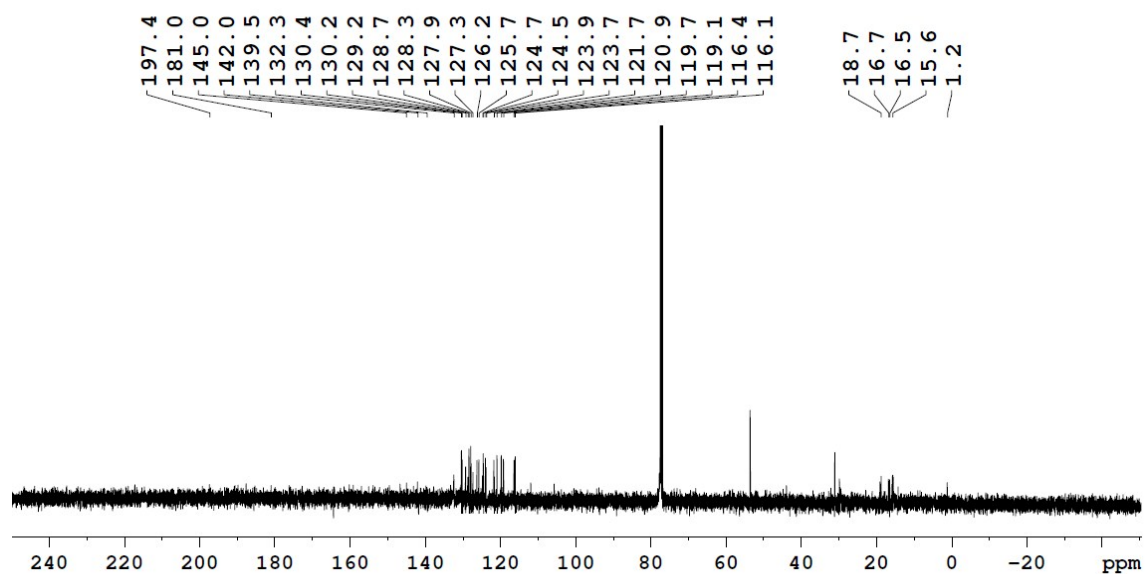


Fig. S35.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **7a**.

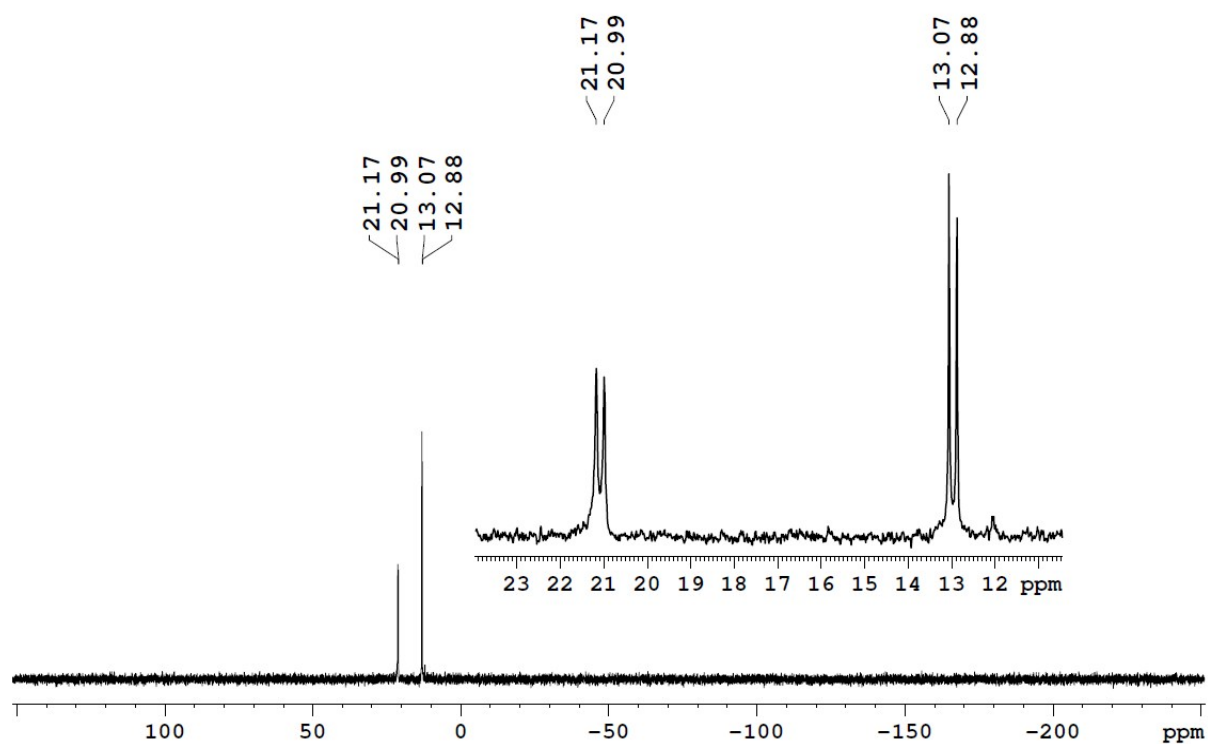
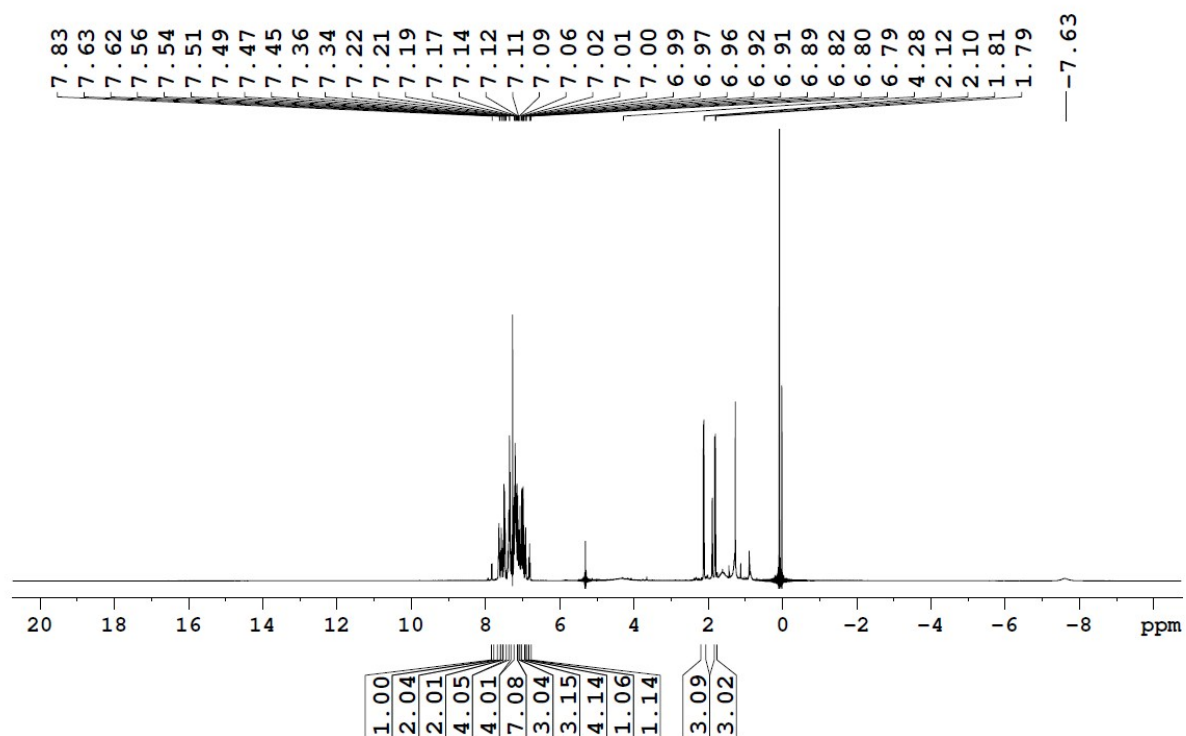
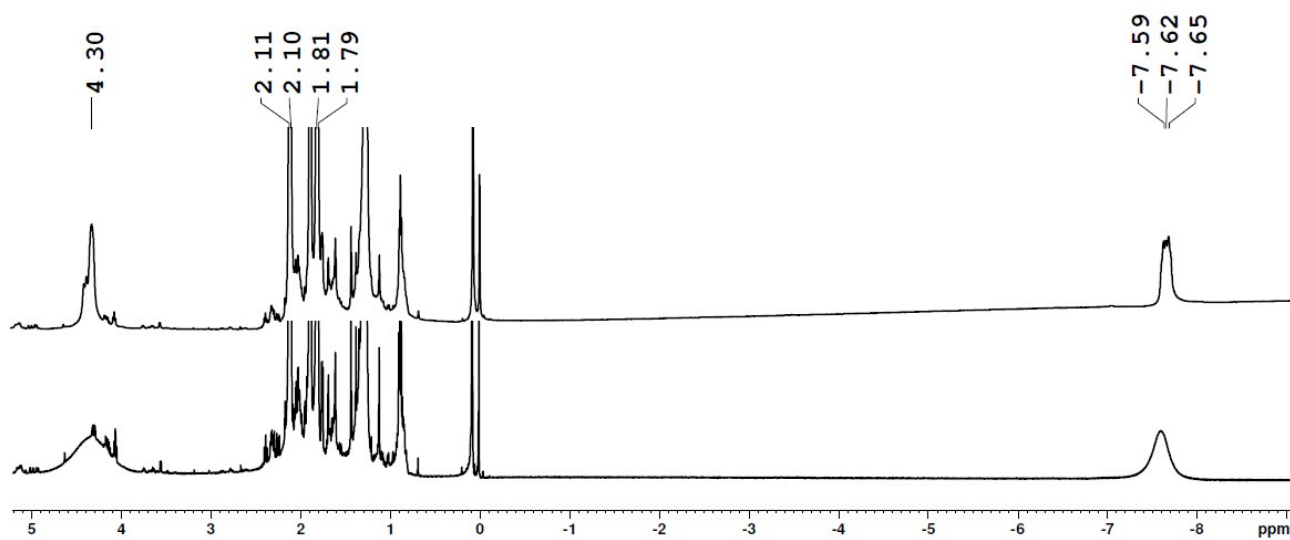


Fig. S36.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **7a**.



**Fig. S37.**  $^1\text{H}$  NMR spectrum of **7b**.



**Fig. S38.** Stacked  $^1\text{H}$  (bottom) and  $^1\text{H}\{^{11}\text{B}\}$  NMR (top) spectrum of **7b**.

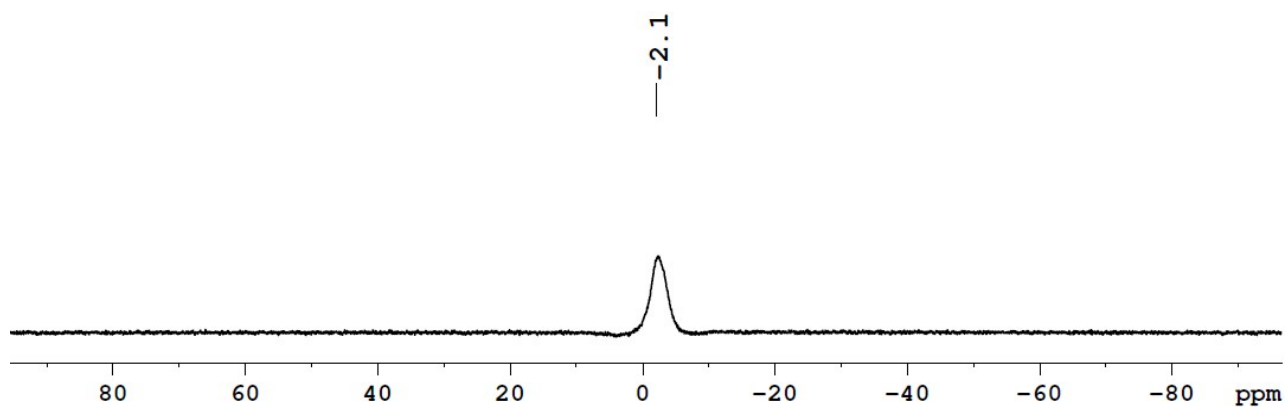


Fig. S39.  $^{11}\text{B}\{^1\text{H}\}$  NMR spectrum of **7b**

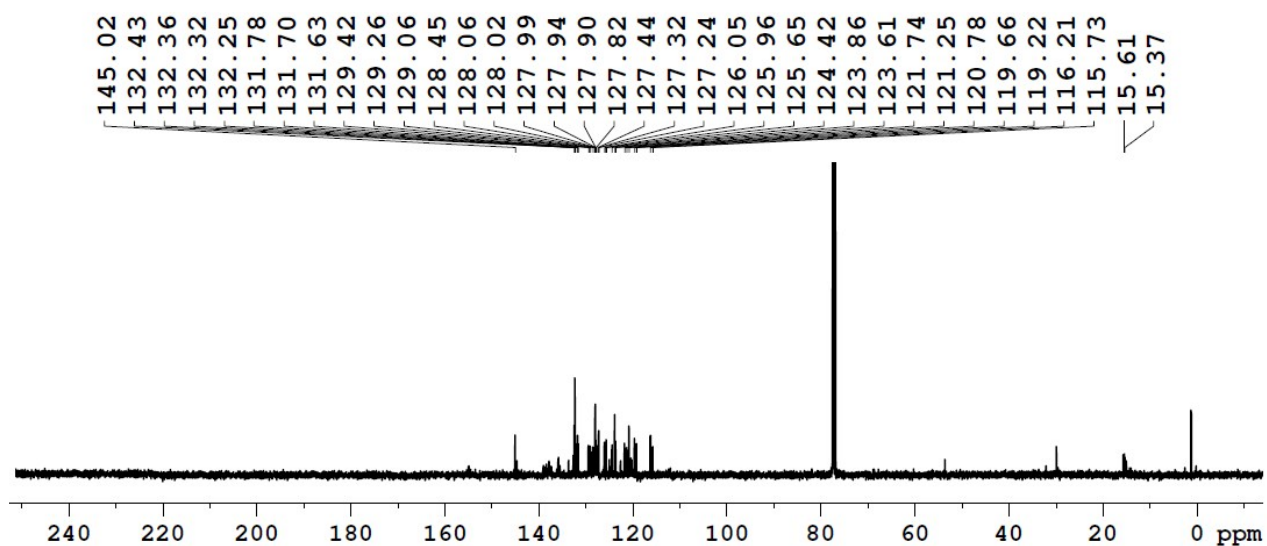
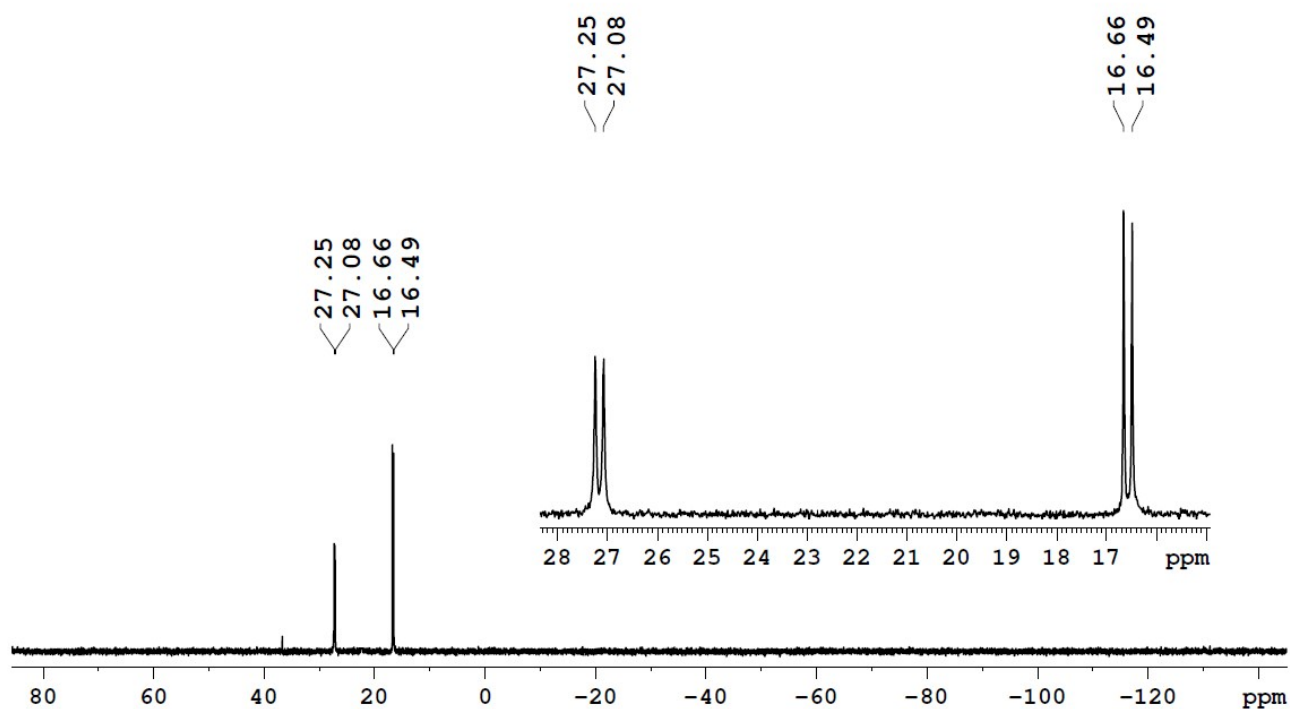
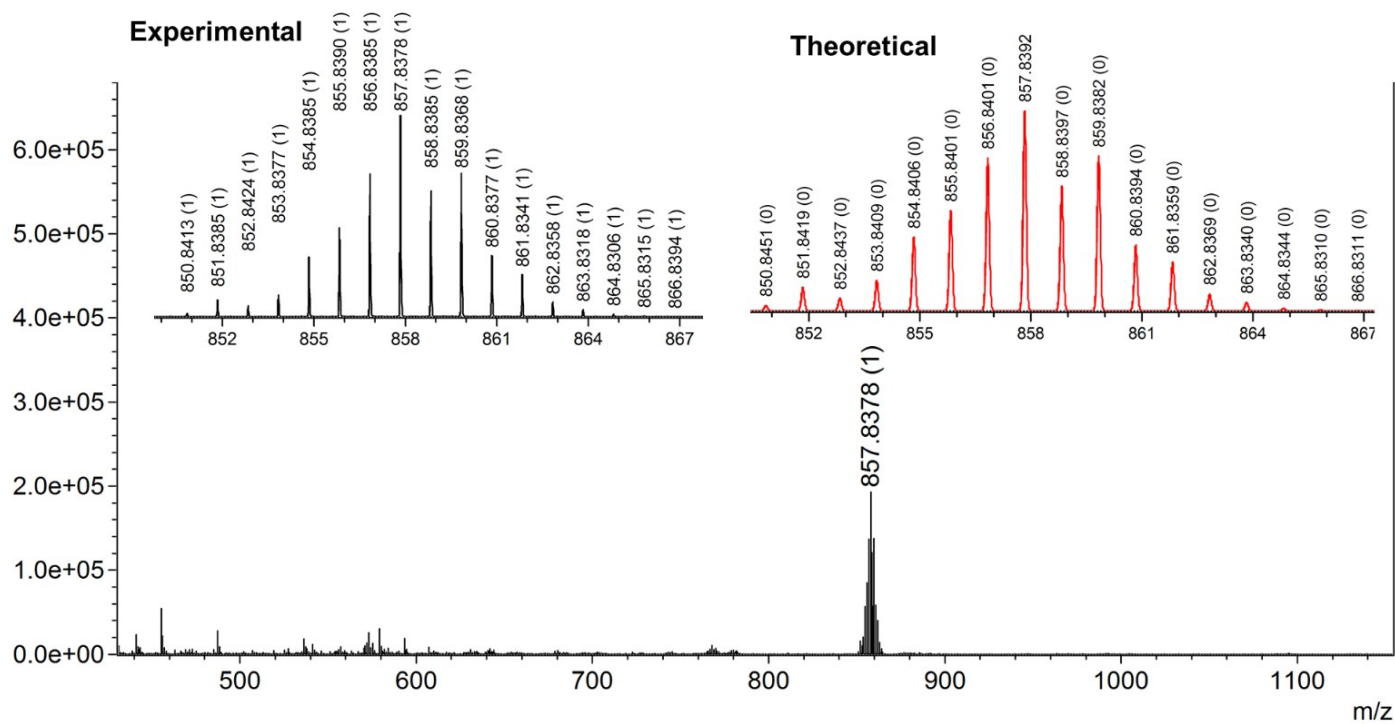


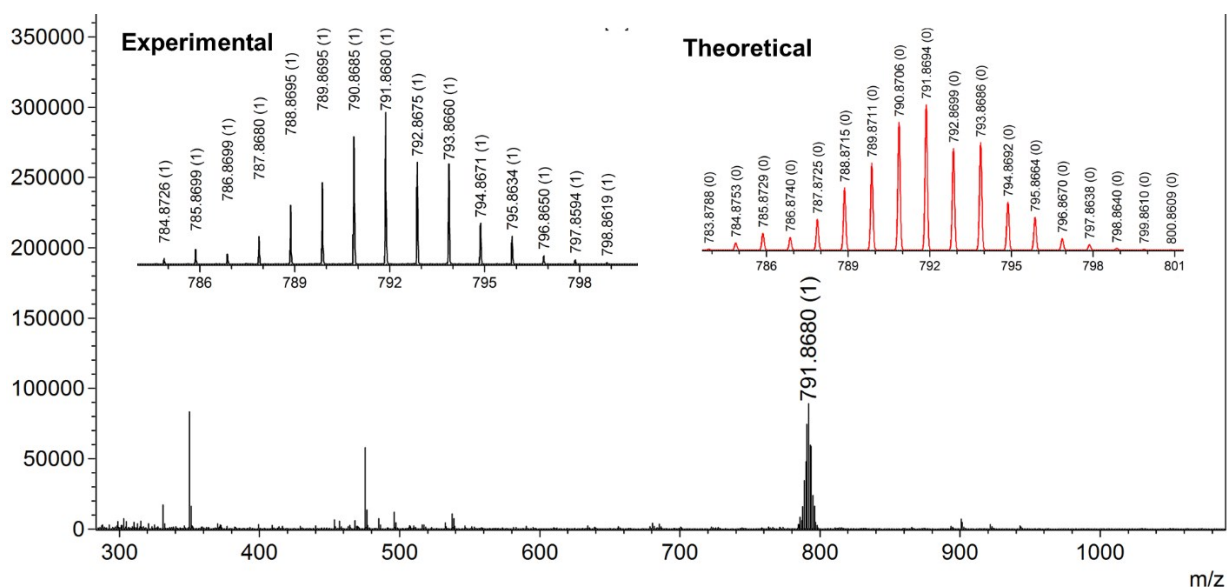
Fig. S40.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **7b**.



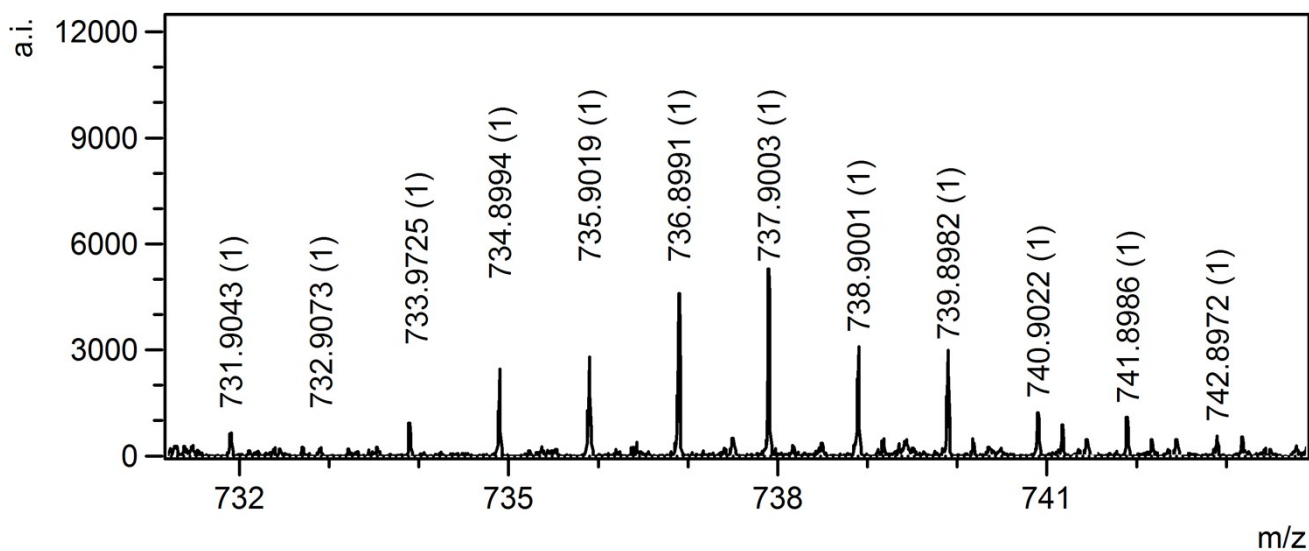
**Fig. S41.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **7b**.



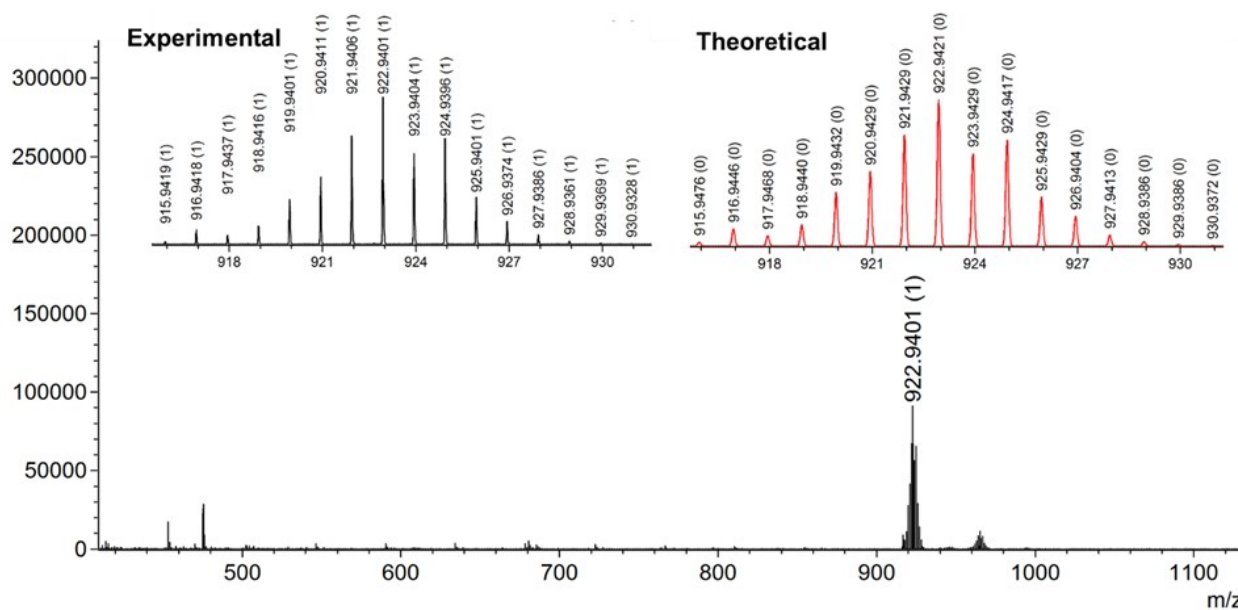
**Fig. S42.** Theoretical (right) and experimental (left) mass spectral isotopic distribution for the fragment of compound **2**.



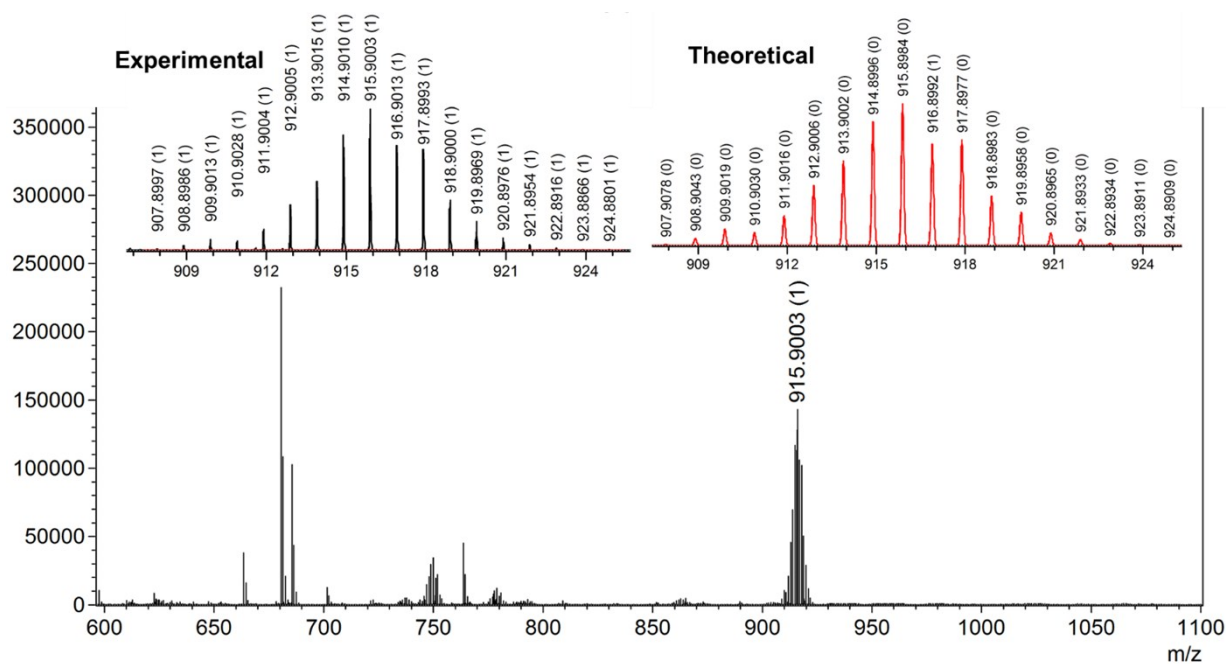
**Fig. S43.** Theoretical (right) and experimental (left) mass spectral isotopic distribution for the fragment of compound **3**.



**Fig. S44.** Experimental mass spectral isotopic distribution for the fragment of compound **4a**.

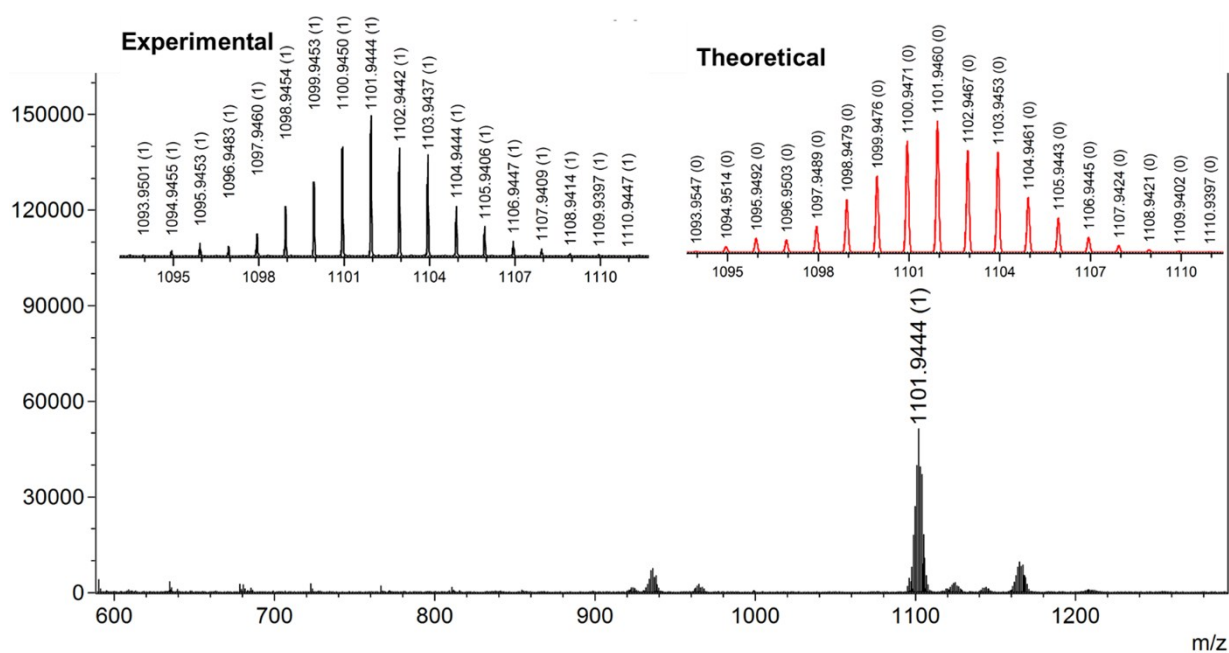


**Fig. S45.** Theoretical (right) and experimental (left) mass spectral isotopic distribution for the fragment of compound **4b**.

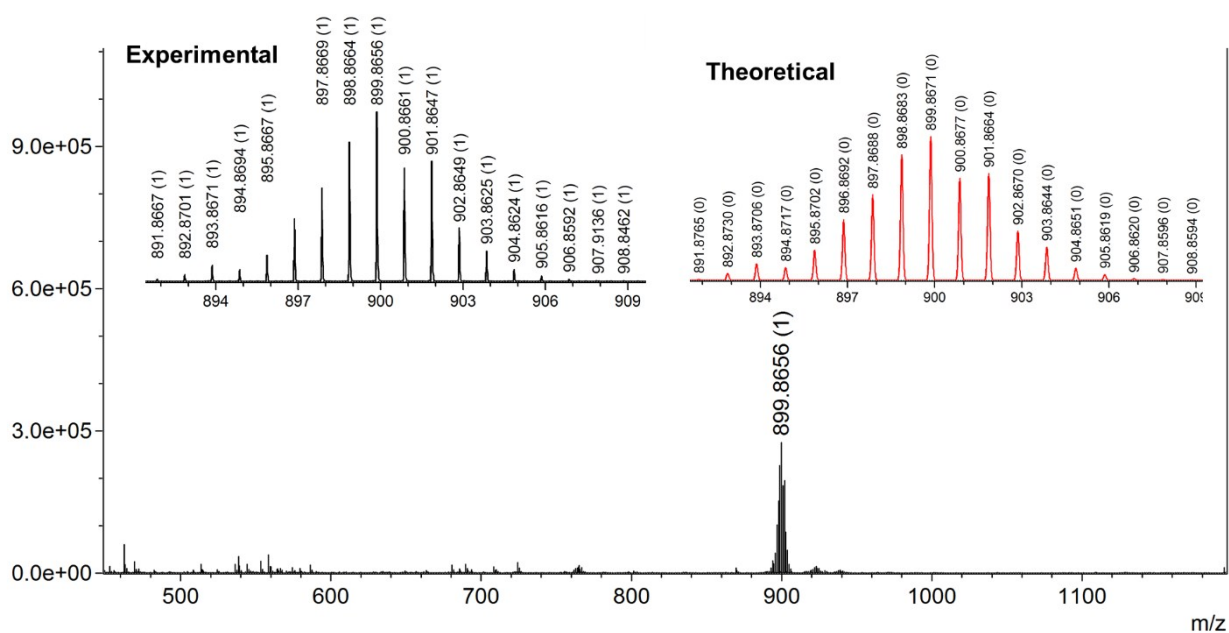


**Fig. S46.** Theoretical (right) and experimental (left) mass spectral isotopic distribution for the fragment of compound **5a**.

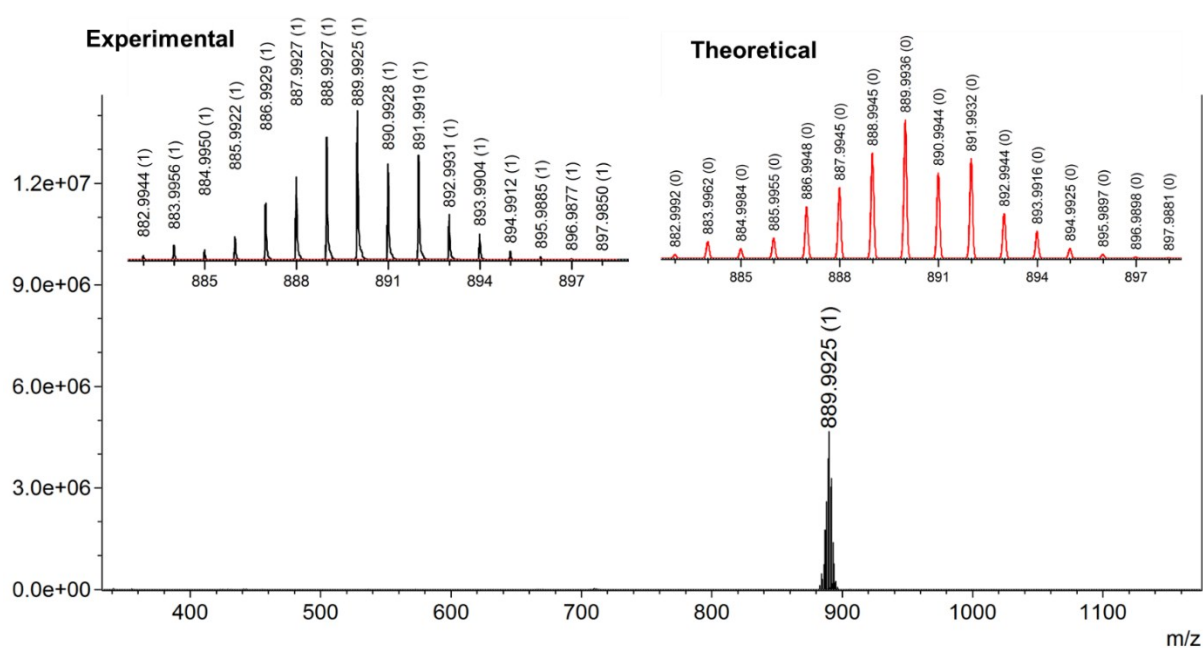




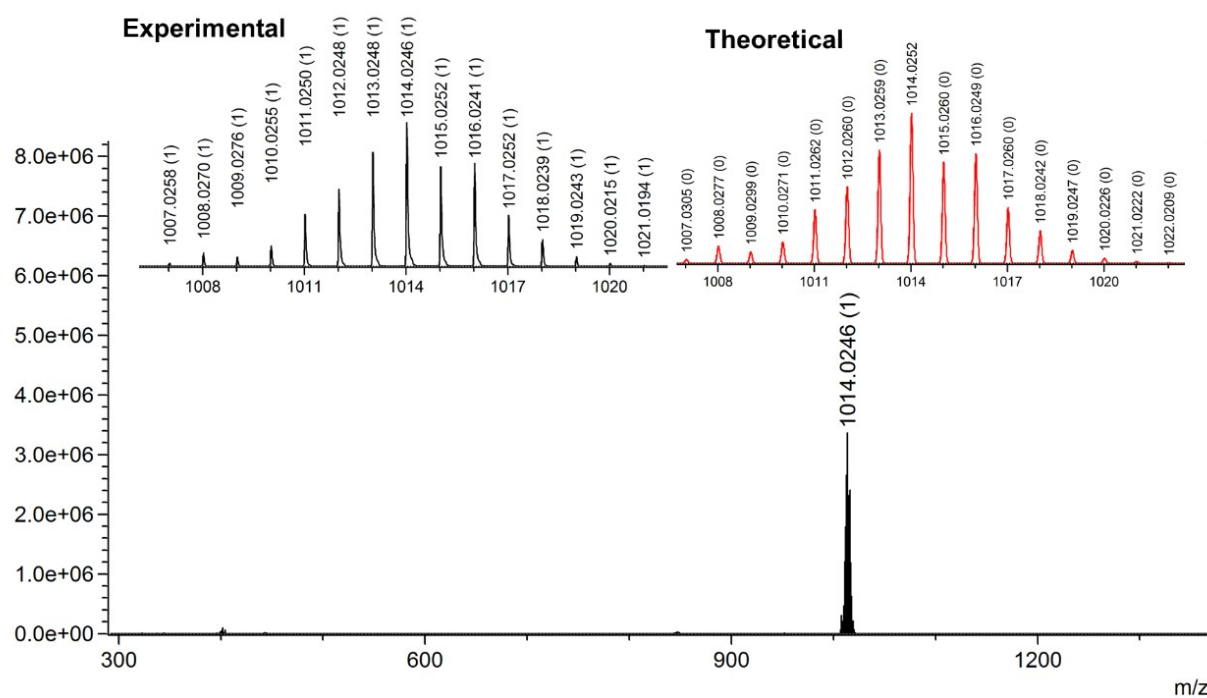
**Fig. S47.** Theoretical (right) and experimental (left) mass spectral isotopic distribution for the fragment of compound **5b**.



**Fig. S48.** Theoretical (right) and experimental (left) mass spectral isotopic distribution for the fragment of compound **6a**.



**Fig. S49.** Theoretical (right) and experimental (left) mass spectral isotopic distribution for the fragment of compound **7a**.



**Fig. S50.** Theoretical (right) and experimental (left) mass spectral isotopic distribution for the fragment of compound **7b**.

## II Computational details

**Table S1.** Selected bond parameters and their Wiberg bond indices (WBI) of **2-7**.

| <b>2</b>  |       |       |       | <b>3</b>           |       |       |       |
|-----------|-------|-------|-------|--------------------|-------|-------|-------|
|           | Expt. | Cal.  | WBI   |                    | Expt. | Cal.  | WBI   |
| Ru2-P11   | 2.210 | 2.211 | 0.752 | Ru1-B1             | 2.644 | 2.637 | 0.159 |
| Ru2-S11   | 2.330 | 2.334 | 0.498 | Ru1-B2             | 2.631 | 2.637 | 0.159 |
| Ru2-S17   | 2.348 | 2.378 | 0.461 | Ru1-S1             | 2.379 | 2.367 | 0.471 |
| Ru2-S15   | 2.423 | 2.414 | 0.440 | Ru1-S3             | 2.300 | 2.316 | 0.577 |
| P11-O91   | 1.504 | 1.527 | 1.093 | Ru1-S5             | 2.369 | 2.367 | 0.471 |
| P11-N88   | 1.803 | 1.820 | 0.570 | Ru1-H <sub>b</sub> | -     | 1.737 | 0.191 |
| Ru2-H59A  | 1.900 | 1.834 | 0.113 | B1-H <sub>b</sub>  | -     | 1.282 | 0.657 |
| B59-H59A  | 1.140 | 1.258 | 0.744 | B1-H <sub>t</sub>  | -     | 1.212 | 0.930 |
| B59-H59B  | 1.130 | 1.208 | 0.939 | B1-N1              | 1.577 | 1.566 | 0.725 |
| <b>4a</b> |       |       |       | <b>4b</b>          |       |       |       |
|           | Expt. | Cal.  | WBI   |                    | Expt. | Cal.  | WBI   |
| Ru1-P1    | -     | 2.203 | 0.795 | Ru1-P1             | 2.270 | 2.187 | 0.808 |
| Ru1-S1    | -     | 2.481 | 0.421 | Ru1-S1             | 2.449 | 2.467 | 0.430 |
| Ru1-S11   | -     | 2.306 | 0.585 | Ru1-S11            | 2.314 | 2.309 | 0.580 |
| Ru1-N32   | -     | 2.153 | 0.340 | Ru1-N32            | 2.130 | 2.156 | 0.342 |
| Ru1-B61   | -     | 2.789 | 0.097 | Ru1-B61            | 2.814 | 2.777 | 0.102 |
| Ru1-H61B  | -     | 1.821 | 0.125 | Ru1-H61B           | 1.975 | 1.816 | 0.131 |
| P1-O1     | -     | 1.637 | 0.733 | P1-O1              | 1.603 | 1.643 | 0.701 |
| B61-H61B  | -     | 1.255 | 0.734 | B61-H61B           | 0.970 | 1.258 | 0.852 |
| B61-H61A  | -     | 1.208 | 0.939 | B61-H61A           | 0.970 | 1.208 | 0.968 |
| B61-N47   | -     | 1.571 | 0.729 | B61-N47            | 1.556 | 1.569 | 0.730 |
| <b>5a</b> |       |       |       | <b>5b</b>          |       |       |       |
|           | Expt. | Cal.  | WBI   |                    | Expt. | Cal.  | WBI   |
| Ru1-P1    | 2.208 | 2.218 | 0.767 | Ru1-P1             | 2.183 | 2.199 | 0.788 |
| Ru1-S1    | 2.418 | 2.423 | 0.429 | Ru1-S5             | 2.362 | 2.383 | 0.464 |
| Ru1-S5    | 2.327 | 2.336 | 0.494 | Ru1-S8             | 2.425 | 2.426 | 0.427 |
| P1-O1     | 1.595 | 1.626 | 0.737 | P1-O1              | 1.604 | 1.629 | 0.723 |
| Ru1-H39A  | 1.973 | 1.824 | 0.123 | Ru1-H2B            | 1.938 | 1.818 | 0.128 |
| B39-H39A  | 0.990 | 1.258 | 0.732 | Ru1-B2             | 2.791 | 2.797 | 0.102 |
| B39-H39B  | 0.990 | 1.207 | 0.936 | B1-H1A             | 0.970 | 1.210 | 0.941 |
| B19-H19A  | 0.990 | 1.200 | 0.946 | B2-H2B             | 0.970 | 1.258 | 0.724 |
| B19-H19B  | 0.990 | 1.210 | 0.941 | B2-H2A             | 0.970 | 1.206 | 0.936 |

| 6a      |       |       |       | 7a       |       |       |       |
|---------|-------|-------|-------|----------|-------|-------|-------|
|         | Expt. | Cal.  | WBI   |          | Expt. | Cal.  | WBI   |
| Ru1-P1  | 2.180 | 2.204 | 0.760 | Ru1-P1   | 2.303 | 2.317 | 0.543 |
| Ru1-S2  | 2.343 | 2.340 | 0.487 | Ru1-P2   | 2.271 | 2.292 | 0.640 |
| Ru1-S6  | 2.364 | 2.370 | 0.463 | Ru1-S1   | 2.409 | 2.415 | 0.455 |
| Ru1-H5X | 1.880 | 1.833 | 0.117 | Ru1-S3   | 2.357 | 2.346 | 0.452 |
| B2-H5X  | 1.150 | 1.257 | 0.737 | Ru1-S5   | 2.471 | 2.458 | 0.360 |
| B2-H6X  | 1.130 | 1.208 | 0.939 | Ru1-H51A | 1.840 | 1.784 | 0.140 |
| P1-O1   | 1.568 | 1.591 | 0.778 | B51-H51A | 1.150 | 1.269 | 0.695 |
| B4-O1   | 1.450 | 1.456 | 0.766 | B51-H51B | 1.130 | 1.207 | 0.932 |
| P1-O2   | 1.618 | 1.633 | 0.737 | B51-N32  | 1.566 | 1.558 | 0.716 |
| 7b      |       |       |       |          |       |       |       |
|         | Expt. | Cal.  | WBI   |          |       |       |       |
| Ru1-P1  | -     | 2.361 | 0.510 |          |       |       |       |
| Ru1-P2  | -     | 2.314 | 0.623 |          |       |       |       |
| Ru1-S1  | -     | 2.411 | 0.458 |          |       |       |       |
| Ru1-S3  | -     | 2.356 | 0.442 |          |       |       |       |
| Ru1-S5  | -     | 2.433 | 0.384 |          |       |       |       |
| Ru1-H1A | -     | 1.777 | 0.145 |          |       |       |       |
| B1-H1A  | -     | 1.273 | 0.681 |          |       |       |       |
| B1-H1B  | -     | 1.206 | 0.931 |          |       |       |       |
| B1-N2   | -     | 1.558 | 0.710 |          |       |       |       |

**Table S2.** Calculated natural charges ( $q_{Ru}$ ,  $q_B$ ,  $q_{Hb}$ ,  $q_P$  and  $q_O$ ) and HOMO – LUMO gaps of **2-7**.

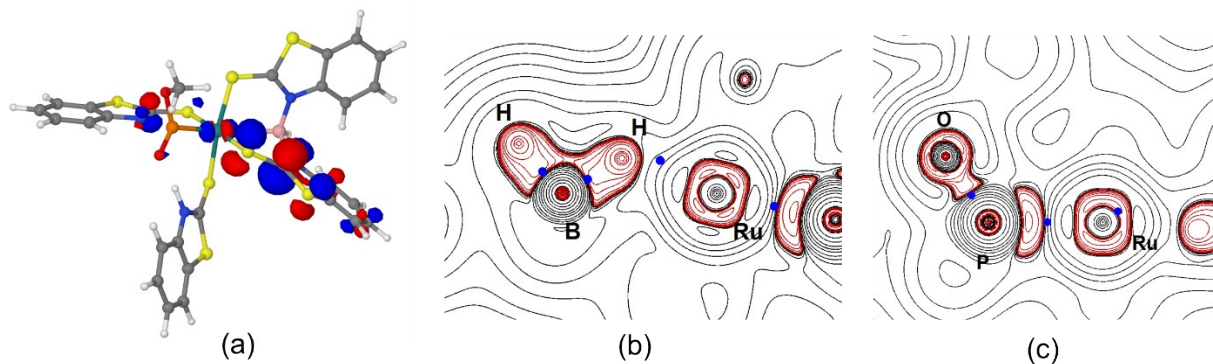
| Molecule  | $q_{Ru}$ | $q_{B1}$ | $q_{B2}$ | $q_{Hb}$ | $q_P$ | $q_O$  | $\Delta E_{H-L}$ (eV) |
|-----------|----------|----------|----------|----------|-------|--------|-----------------------|
| <b>2</b>  | -0.629   | 0.230    | -        | -0.005   | 1.960 | -1.095 | 1.854                 |
| <b>3</b>  | -0.463   | 0.243    | 0.243    | 0.058    | -     | -      | 1.888                 |
| <b>4a</b> | -0.423   | 0.235    | -        | -0.002   | 2.015 | -0.769 | 1.862                 |
| <b>4b</b> | -0.407   | 0.237    | -        | 0.002    | 2.014 | -0.736 | 1.822                 |
| <b>5a</b> | -0.578   | 0.238    | 0.115    | 0.002    | 2.034 | -0.770 | 1.694                 |
| <b>5b</b> | -0.567   | 0.245    | 0.113    | 0.001    | 2.031 | -0.746 | 1.686                 |
| <b>6a</b> | -0.627   | 0.228    | 0.623    | 0.002    | 2.058 | -0.937 | 1.803                 |
| <b>7a</b> | -0.650   | 0.263    | -        | 0.022    | 1.274 | -      | 1.726                 |
| <b>7b</b> | -0.626   | 0.277    | -        | 0.027    | 1.247 | -      | 1.644                 |

**Table S3.** Experimentally observed and calculated  $^{11}\text{B}\{^1\text{H}\}$  and  $^1\text{H}$  chemical shifts of **2-7**.

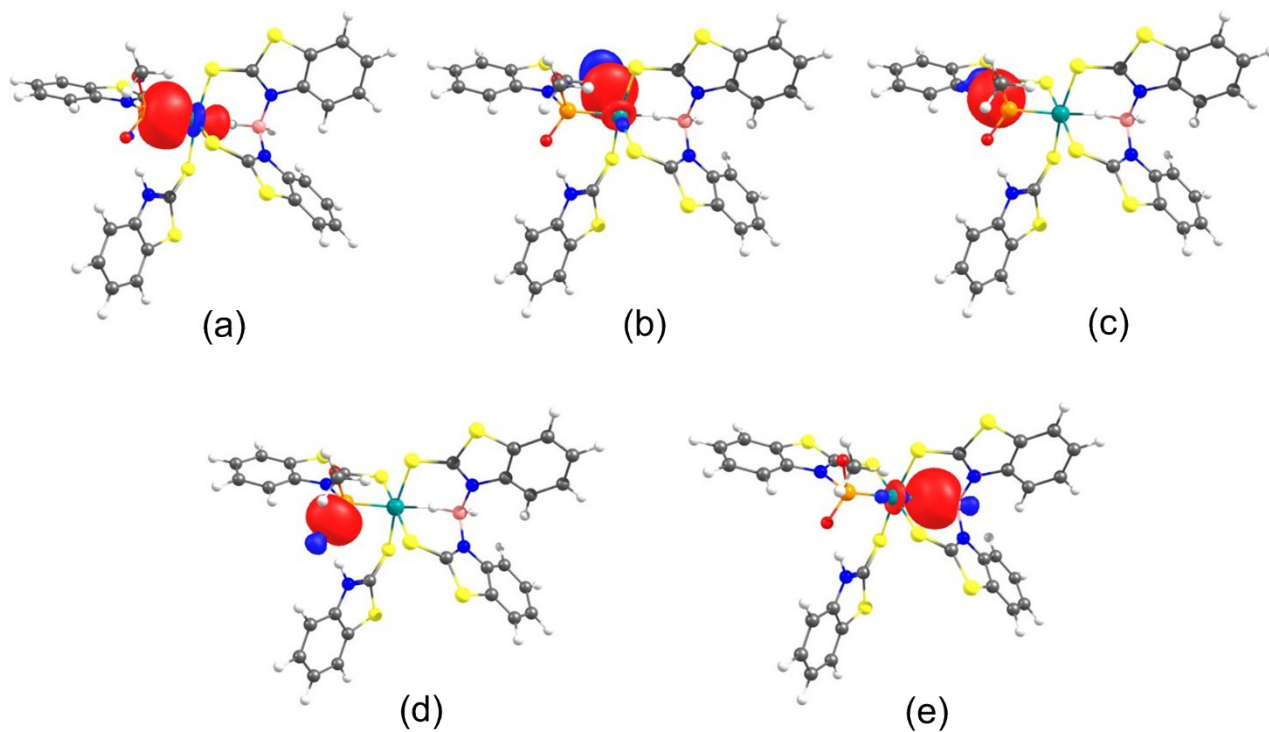
| Molecule  |    | $^{11}\text{B}$ NMR |       |                  | $^1\text{H}$ NMR |       |
|-----------|----|---------------------|-------|------------------|------------------|-------|
|           |    | Exp.                | Cal.  |                  | Exp.             | Cal.  |
| <b>2</b>  | B1 | -4.0                | -7.2  | B-H <sub>b</sub> | -3.40            | -1.65 |
|           |    |                     |       | B-H <sub>t</sub> | 3.96             | 5.55  |
| <b>3</b>  | B1 | -4.8                | -7.4  | B-H <sub>b</sub> | -11.94           | -8.30 |
|           |    |                     |       | B-H <sub>t</sub> | 4.59             | 5.16  |
| <b>4a</b> | B1 | -4.0                | -7.0  | B-H <sub>b</sub> | -2.32            | -1.96 |
|           |    |                     |       | B-H <sub>t</sub> | 4.78             | 5.14  |
| <b>4b</b> | B1 | -3.7                | -6.5  | B-H <sub>b</sub> | -2.44            | -1.89 |
|           |    |                     |       | B-H <sub>t</sub> | 4.72             | 5.20  |
| <b>5a</b> | B1 | -3.1                | -4.8  | B-H <sub>b</sub> | -4.13            | -2.77 |
|           | B2 | -6.3                | -14.3 | B-H <sub>t</sub> | 4.31             | 5.07  |
| <b>5b</b> | B1 | -3.3                | -4.9  | B-H <sub>b</sub> | -4.44            | -2.92 |
|           | B2 | -6.8                | -14.4 | B-H <sub>t</sub> | 4.38             | 5.14  |
| <b>6a</b> | B1 | 0.1                 | -3.4  | B-H <sub>b</sub> | -3.15            | -2.97 |
|           | B2 | -4.6                | -7.5  | B-H <sub>t</sub> | 4.78             | 5.13  |
| <b>7a</b> | B1 | -2.9                | -5.4  | B-H <sub>b</sub> | -6.93            | -5.20 |
|           |    |                     |       | B-H <sub>t</sub> | 4.51             | 5.50  |
| <b>7b</b> | B1 | -2.1                | -3.4  | B-H <sub>b</sub> | -7.63            | -5.74 |
|           |    |                     |       | B-H <sub>t</sub> | 4.28             | 5.58  |

**Table S4.** Electron density,  $\rho(r)$ , Lagrangian kinetic energy,  $G(r)$ , Potential energy density,  $V(r)$ , Total energy density,  $H(r)$ , Laplacian of the electron density,  $\nabla^2\rho(r)$ , Electron localization function, ELF and Ellipticity,  $\epsilon$  in a.u of selected bond critical points (bcps) in **2-7** at the PE0/def2-TZVP level of theory.

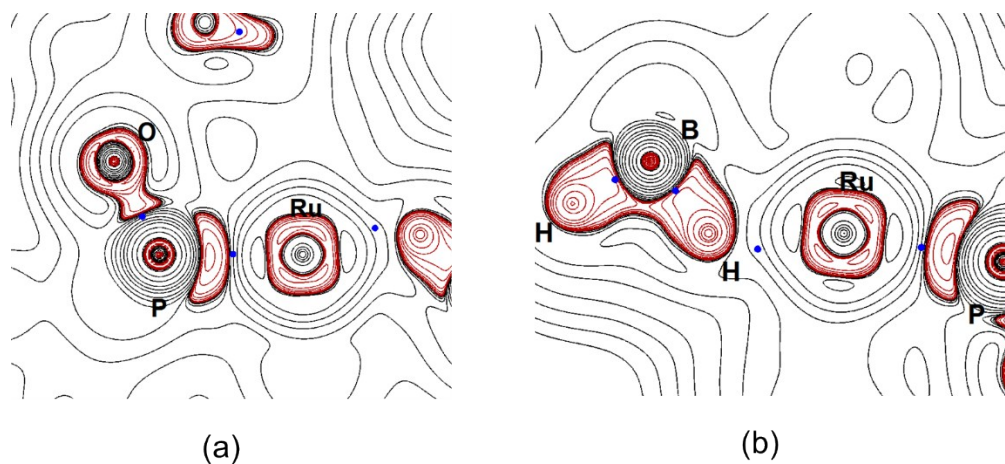
|           | BCP                | $\rho(r)$ | $G(r)$ | $V(r)$ | $H(r)$ | $\nabla^2\rho(r)$ | ELF   | $\epsilon$ |
|-----------|--------------------|-----------|--------|--------|--------|-------------------|-------|------------|
| <b>2</b>  | Ru2-P11            | 0.120     | 0.099  | -0.155 | -0.055 | 0.175             | 0.415 | 2.791      |
|           | Ru2-S15            | 0.213     | 0.113  | -0.331 | -0.218 | 0.420             | 0.790 | 0.303      |
|           | Ru2-H59A           | 0.040     | 0.077  | -0.084 | -0.007 | 0.280             | 0.030 | 5.925      |
|           | P11-O91            | 0.210     | 0.340  | -0.487 | -0.146 | 0.778             | 0.281 | 2.485      |
|           | P11-N88            | 0.131     | 0.127  | -0.228 | -0.100 | 0.106             | 0.367 | 1.345      |
|           | B59-H59A           | 0.169     | 0.126  | -0.305 | -0.179 | -0.211            | 0.579 | 0.221      |
|           | B59-H59B           | 0.184     | 0.105  | -0.312 | -0.207 | -0.408            | 0.725 | 0.114      |
| <b>3</b>  | Ru1-H <sub>b</sub> | 0.050     | 0.105  | -0.116 | -0.011 | 0.377             | 0.034 | 5.419      |
|           | Ru1-H <sub>b</sub> | 0.050     | 0.106  | -0.117 | -0.011 | 0.379             | 0.033 | 5.889      |
|           | Ru1-S1             | 0.084     | 0.082  | -0.109 | -0.026 | 0.222             | 0.245 | 6.452      |
|           | B1-H <sub>b</sub>  | 0.162     | 0.114  | -0.283 | -0.169 | -0.220            | 0.594 | 0.107      |
|           | B2-H <sub>b</sub>  | 0.162     | 0.114  | -0.284 | -0.169 | -0.217            | 0.592 | 0.115      |
|           | B1-H <sub>t</sub>  | 0.183     | 0.102  | -0.307 | -0.204 | -0.407            | 0.731 | 0.134      |
| <b>6a</b> | Ru1-P1             | 0.121     | 0.102  | -0.160 | -0.057 | 0.180             | 0.412 | 2.776      |
|           | Ru1-S2             | 0.089     | 0.084  | -0.113 | -0.029 | 0.217             | 0.271 | 4.722      |
|           | Ru1-H5X            | 0.039     | 0.076  | -0.083 | -0.006 | 0.280             | 0.029 | 6.122      |
|           | P1-O1              | 0.183     | 0.266  | -0.397 | -0.130 | 0.543             | 0.289 | 2.212      |
|           | P1-O3              | 0.167     | 0.230  | -0.350 | -0.119 | 0.447             | 0.287 | 2.115      |
|           | O1-B4              | 0.158     | 0.262  | -0.381 | -0.119 | 0.572             | 0.204 | 2.248      |
|           | B4-H4X             | 0.188     | 0.099  | -0.313 | -0.213 | -0.457            | 0.761 | 0.007      |
|           | B2-H5X             | 0.170     | 0.127  | -0.308 | -0.181 | -0.215            | 0.582 | 0.217      |
|           | B2-H6X             | 0.184     | 0.105  | -0.311 | -0.206 | -0.404            | 0.725 | 0.118      |



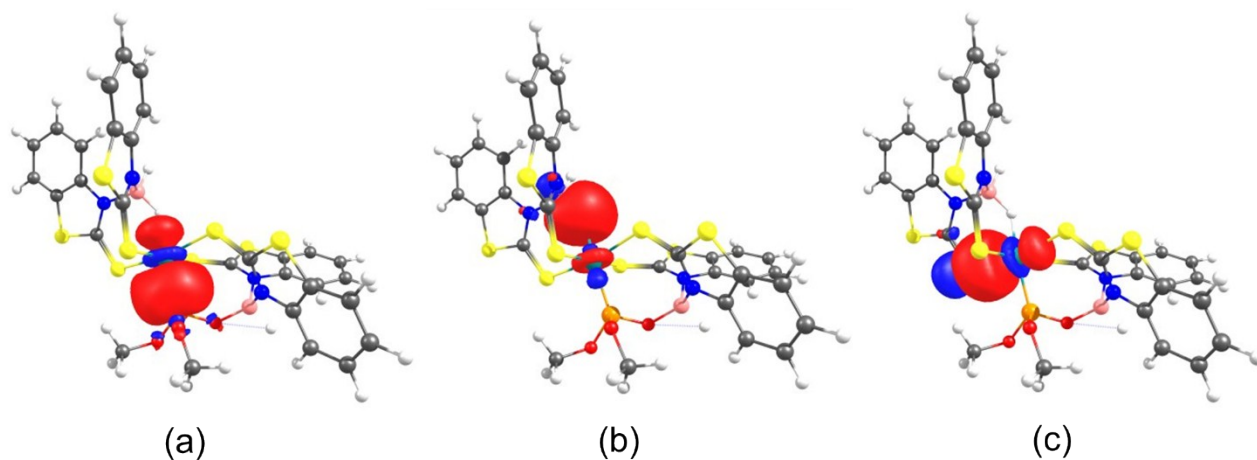
**Fig. S51.** LUMO of **2** (a); contour plot of Laplacian of the electron density,  $\nabla^2\rho(r)$  with negative contours shown as red lines and positive contours shown as black lines for **2** in Ru-H-B plane (b) and Ru-P-O plane (c) (blue dots indicates *bcps*).



**Fig. S52.** Selected bonding diagrams of **2** as obtained from NBO analysis [Ru2-P11 bond (a), Ru2-S17 bond (b), P11-N88 bond (c), P11-O91 bond (d) and Ru2-H59A-B59 bond (e)]. Isosurfaces are plotted at an isovalue of  $0.04 \text{ [e/bohr}^3\text{]}^{1/2}$ .

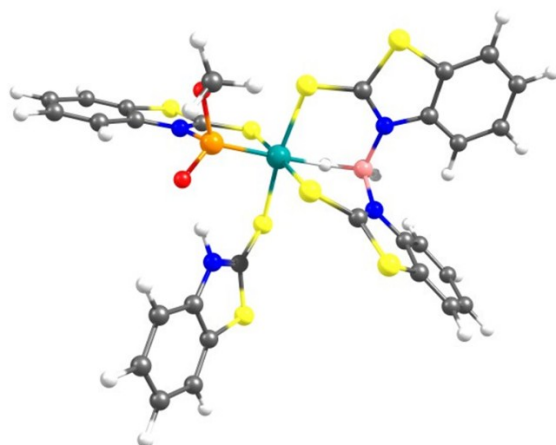


**Fig. S53.** contour plot of Laplacian of the electron density,  $\nabla^2\rho(r)$  with negative contours shown as red lines and positive contours shown as black lines for **6a** in Ru-P-O plane (a) and Ru-H-B plane (b) (blue dots indicates *bcps*).



**Fig. S54.** Selected bonding diagrams of **6a** as obtained from NBO analysis [Ru1-P1 bond (a), Ru1-H5X-B2 bond (b), and Ru1-S2 bond (c)].



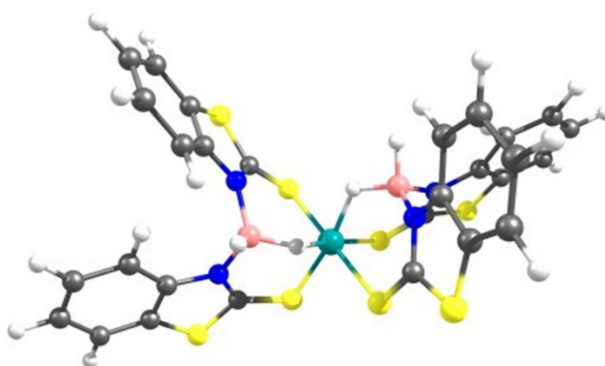


**Fig. 55.** Optimized geometry of **2**.

T. E. = -5132.20937993 a. u.

Cartesian coordinates for the calculated structure of **2** (in Å).

|    |             |             |             |   |            |             |             |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| H  | 2.36474200  | 1.63172300  | 0.81288600  | S | 1.26948500 | 4.09360800  | -1.57071600 |
| Ru | 0.15854100  | -0.75080000 | -0.20093100 | C | 1.38161800 | 2.49265800  | -0.84230100 |
| S  | -0.68922300 | -2.64811700 | 0.86168700  | C | 2.23366800 | 4.79209200  | -0.28827500 |
| S  | -3.34362700 | -3.78024900 | 1.47466300  | C | 2.64921000 | 6.11228200  | -0.11175500 |
| C  | -2.36470100 | -2.56135500 | 0.68143900  | H | 2.38287700 | 6.88478800  | -0.83397200 |
| C  | -4.79593600 | -3.11407700 | 0.78049500  | C | 3.41445100 | 6.41904600  | 1.01550000  |
| C  | -6.10603200 | -3.56891500 | 0.92828100  | H | 3.74708800 | 7.44585800  | 1.17282600  |
| H  | -6.32444300 | -4.44389800 | 1.54172300  | C | 3.75979800 | 5.42491200  | 1.94304300  |
| C  | -7.12547200 | -2.87982600 | 0.27075600  | H | 4.36069300 | 5.68809900  | 2.81469300  |
| H  | -8.15776400 | -3.21695200 | 0.37286500  | C | 3.34864500 | 4.10400100  | 1.77158800  |
| C  | -6.82616300 | -1.76163600 | -0.51666200 | H | 3.61532800 | 3.32416400  | 2.48577400  |
| H  | -7.62973700 | -1.22881100 | -1.02722300 | C | 2.57912800 | 3.79130900  | 0.64571600  |
| C  | -5.51507000 | -1.30714900 | -0.66280500 | N | 2.08788600 | 2.54566200  | 0.30146700  |
| H  | -5.30473400 | -0.43410900 | -1.27555000 | S | 1.08835400 | -2.10222100 | -1.92298400 |
| C  | -4.48128700 | -1.98684000 | -0.00871300 | S | 3.91954300 | -3.04322200 | -2.44209700 |
| N  | -3.10948500 | -1.68376000 | -0.04433800 | C | 2.70799200 | -2.22657300 | -1.48197600 |
| B  | -2.53389500 | -0.52662800 | -0.93861700 | C | 5.15835300 | -2.67832000 | -1.25663000 |
| H  | -1.33761600 | -0.74660500 | -1.26167000 | C | 6.51203600 | -3.01298500 | -1.28825400 |
| H  | -3.06911900 | -0.58044100 | -2.02095400 | H | 6.92881200 | -3.58024500 | -2.12122500 |
| S  | -0.74130700 | 0.65863900  | 1.47602000  | C | 7.31694700 | -2.60144600 | -0.22477900 |
| S  | -2.89374900 | 2.73393200  | 1.50208300  | H | 8.37857300 | -2.85206500 | -0.22788700 |
| C  | -2.14456000 | 1.31031400  | 0.80787100  | C | 6.77445300 | -1.86887700 | 0.83995700  |
| C  | -3.99542300 | 2.84613100  | 0.15230000  | H | 7.42151000 | -1.55159400 | 1.65904200  |
| C  | -4.95461000 | 3.82853400  | -0.09316700 | C | 5.42154100 | -1.53253500 | 0.87606200  |
| H  | -5.12676400 | 4.62995900  | 0.62630700  | H | 4.99537200 | -0.94706200 | 1.68920800  |
| C  | -5.67220700 | 3.77170400  | -1.28842400 | C | 4.60816400 | -1.94653200 | -0.18378700 |
| H  | -6.42180300 | 4.53397300  | -1.50439400 | N | 3.23801600 | -1.71423400 | -0.34205700 |
| C  | -5.41620800 | 2.75593800  | -2.21813800 | P | 2.10572100 | -0.90989700 | 0.83526900  |
| H  | -5.96168500 | 2.73832400  | -3.16284200 | O | 2.27073500 | -2.12135800 | 1.93549300  |
| C  | -4.46566000 | 1.76570800  | -1.96688200 | C | 1.83777100 | -1.86316500 | 3.28258600  |
| H  | -4.25361600 | 0.99498400  | -2.70675800 | H | 2.32277800 | -0.96006100 | 3.68182600  |
| C  | -3.75885100 | 1.79129500  | -0.75717500 | H | 2.13320600 | -2.73801400 | 3.87479200  |
| N  | -2.77286400 | 0.89337400  | -0.32373300 | H | 0.74284500 | -1.74818100 | 3.32742500  |
| S  | 0.68259800  | 1.14943100  | -1.59487500 | O | 2.85847500 | 0.29919400  | 1.38613400  |

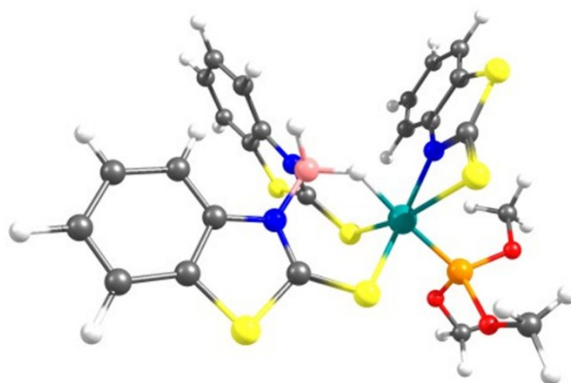


**Fig. S6.** Optimized geometry of **3**.

T. E. = -4626.12398691 a. u.

Cartesian coordinates for the calculated structure of **2** (in Å).

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Ru | 0.00001600  | -1.23232000 | -0.00000200 | C | -6.41309900 | 1.06295900  | 1.32603300  |
| S  | -1.03408700 | -1.24648500 | -2.12971000 | H | -6.85324600 | 2.06094000  | 1.30171600  |
| S  | -2.58774300 | 0.85954400  | -3.61571200 | C | -5.06308900 | 0.91245700  | 1.00669500  |
| S  | -1.46263300 | -2.85819200 | 0.76339700  | H | -4.46622300 | 1.77978400  | 0.73629000  |
| S  | -4.36517000 | -2.93425800 | 1.36937700  | C | -4.49412700 | -0.36579800 | 1.03580500  |
| S  | 1.03413000  | -1.24641000 | 2.12972100  | C | 1.95380100  | 0.16178900  | 2.14051300  |
| S  | 2.58767300  | 0.85974400  | 3.61566200  | C | 3.08951600  | 2.29376400  | 2.75184400  |
| S  | 1.46268000  | -2.85820500 | -0.76334900 | C | 3.67165700  | 3.44960500  | 3.27179900  |
| S  | 4.36522800  | -2.93427500 | -1.36928000 | H | 3.91405400  | 3.52117900  | 4.33279500  |
| N  | -2.21334700 | 0.93057600  | -1.04872100 | C | 3.91843100  | 4.51625700  | 2.40628400  |
| N  | -3.16167800 | -0.71258200 | 0.75360400  | H | 4.36726600  | 5.43180300  | 2.79340700  |
| N  | 2.21333900  | 0.93064600  | 1.04866000  | C | 3.57182700  | 4.42241900  | 1.05251100  |
| N  | 3.16171500  | -0.71259000 | -0.75357300 | H | 3.74279000  | 5.27302400  | 0.39104000  |
| B  | -2.06417200 | 0.35964100  | 0.40226400  | C | 3.00043800  | 3.26173400  | 0.52949000  |
| B  | 2.06419600  | 0.35964000  | -0.40230400 | H | 2.71167700  | 3.20533200  | -0.51956900 |
| C  | -1.95381200 | 0.16167700  | -2.14054700 | C | 2.77548800  | 2.17085500  | 1.37979100  |
| C  | -3.08961600 | 2.29358500  | -2.75194500 | C | 2.92923900  | -2.04260000 | -0.91380300 |
| C  | -3.67181200 | 3.44938100  | -3.27193800 | C | 5.30446700  | -1.46618800 | -1.39029400 |
| H  | -3.91423800 | 3.52089700  | -4.33293200 | C | 6.65436800  | -1.31791900 | -1.70686900 |
| C  | -3.91860600 | 4.51606200  | -2.40646500 | H | 7.25957200  | -2.18354900 | -1.97885100 |
| H  | -4.36748600 | 5.43157300  | -2.79361700 | C | 7.20691600  | -0.03732800 | -1.67093300 |
| C  | -3.57196400 | 4.42229800  | -1.05269700 | H | 8.26089900  | 0.10280800  | -1.91410700 |
| H  | -3.74294300 | 5.27292600  | -0.39125900 | C | 6.41315700  | 1.06294100  | -1.32591200 |
| C  | -3.00052100 | 3.26165800  | -0.52963700 | H | 6.85330500  | 2.06092200  | -1.30158600 |
| H  | -2.71173500 | 3.20531200  | 0.51941800  | C | 5.06313600  | 0.91244500  | -1.00662000 |
| C  | -2.77555100 | 2.17074800  | -1.37989400 | H | 4.46626500  | 1.77977600  | -0.73623900 |
| C  | -2.92919400 | -2.04258900 | 0.91385200  | C | 4.49417300  | -0.36580900 | -1.03574000 |
| C  | -5.30440900 | -1.46617200 | 1.39040200  | H | -0.87426800 | 0.05576600  | 0.77243000  |
| C  | -6.65429900 | -1.31789800 | 1.70702300  | H | -2.18921600 | 1.27910000  | 1.18218200  |
| H  | -7.25949300 | -2.18352300 | 1.97903700  | H | 0.87428700  | 0.05576700  | -0.77245600 |
| C  | -7.20684600 | -0.03730600 | 1.67109300  | H | 2.18925300  | 1.27906500  | -1.18226000 |
| H  | -8.26082000 | 0.10283300  | 1.91430200  |   |             |             |             |

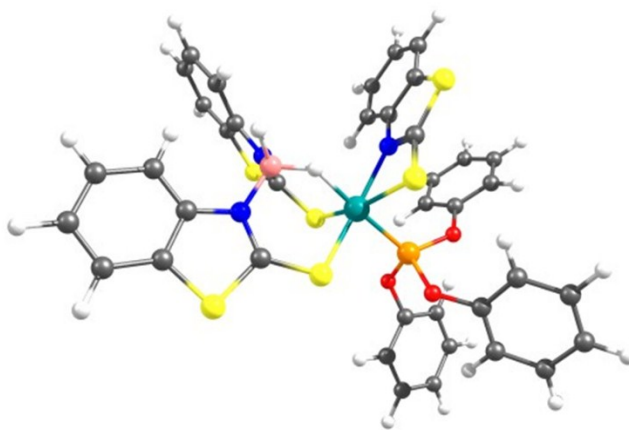


**Fig. S7.** Optimized geometry of **4a**.

T. E. = -4166.74975042 a. u.

Cartesian coordinates for the calculated structure of **4a** (in Å).

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Ru | -0.97977000 | -0.81572000 | -0.13286500 | N | 2.36082200  | -1.20400500 | -0.57283800 |
| P  | -2.70647300 | -1.80614300 | 0.81302200  | C | 1.80952400  | -2.40566800 | -0.24825400 |
| O  | -4.23558200 | -1.29041700 | 0.53224000  | S | -0.14397000 | -0.09822300 | 1.93017100  |
| O  | -2.97334200 | -3.38186400 | 0.51196200  | S | 1.79251700  | 2.00880100  | 2.79829700  |
| O  | -2.59374100 | -1.87722600 | 2.42812500  | C | 1.12964200  | 0.94651600  | 1.56880900  |
| S  | -1.98619000 | -0.99737700 | -2.39436100 | N | 1.69529200  | 1.15264500  | 0.34826600  |
| S  | -3.06715100 | 1.91354300  | -2.93038100 | C | 2.54054400  | 2.27186900  | 0.32524800  |
| C  | -2.33811300 | 0.62141100  | -1.98675400 | C | 3.12860200  | 2.87289600  | -0.79537300 |
| N  | -1.97876800 | 0.98748800  | -0.75673000 | H | 2.92920800  | 2.48184100  | -1.79240200 |
| C  | -2.24719800 | 2.31503700  | -0.48563900 | C | 3.94146700  | 3.99294700  | -0.61673000 |
| C  | -1.99662500 | 3.00125900  | 0.71172300  | H | 4.39427200  | 4.46353900  | -1.49069300 |
| H  | -1.52875100 | 2.47567800  | 1.54505500  | C | 4.17479400  | 4.52603900  | 0.65690700  |
| C  | -2.35361300 | 4.34514600  | 0.80308900  | H | 4.81674300  | 5.39987800  | 0.77463700  |
| H  | -2.15919100 | 4.88723100  | 1.72997600  | C | 3.56888800  | 3.95884600  | 1.77897300  |
| C  | -2.95636300 | 5.01271400  | -0.27426000 | H | 3.72093000  | 4.38275800  | 2.77233400  |
| H  | -3.22599700 | 6.06545400  | -0.17914100 | C | 2.74591400  | 2.84744300  | 1.59851200  |
| C  | -3.21669800 | 4.34359000  | -1.47162900 | B | 1.55576600  | 0.12221300  | -0.82060700 |
| H  | -3.68687600 | 4.86045500  | -2.30934400 | H | 1.95712400  | 0.62862900  | -1.84205400 |
| C  | -2.85949400 | 2.99838900  | -1.57027700 | H | 0.36603600  | -0.11785600 | -1.14201400 |
| S  | 0.18590100  | -2.80212000 | -0.01453500 | C | -4.62376900 | 0.06615300  | 0.81111000  |
| S  | 3.00087300  | -3.68613400 | -0.12964900 | H | -3.84505300 | 0.61515400  | 1.35874400  |
| C  | 4.27564000  | -2.58335700 | -0.57199700 | H | -4.83463900 | 0.58540600  | -0.13367900 |
| C  | 5.63328600  | -2.86047500 | -0.72918500 | H | -5.53769800 | 0.03158400  | 1.42097500  |
| H  | 6.01580600  | -3.86986800 | -0.57300200 | C | -3.21047300 | -3.87896400 | -0.81576400 |
| C  | 6.48595500  | -1.81721300 | -1.09202500 | H | -3.43692800 | -4.94676700 | -0.70470400 |
| H  | 7.55194400  | -2.01041300 | -1.21862200 | H | -4.06090000 | -3.36273900 | -1.28277200 |
| C  | 5.97649000  | -0.52901100 | -1.29261100 | H | -2.31450600 | -3.75687700 | -1.44116100 |
| H  | 6.65008800  | 0.28106700  | -1.57606900 | C | -3.54241400 | -2.61534900 | 3.22441400  |
| C  | 4.61779600  | -0.25304900 | -1.13384000 | H | -3.39065300 | -2.29179000 | 4.26131700  |
| H  | 4.24335900  | 0.75566200  | -1.28790500 | H | -4.57460300 | -2.39833400 | 2.91302400  |
| C  | 3.74951000  | -1.28816900 | -0.76897900 | H | -3.35310500 | -3.69359600 | 3.13631300  |



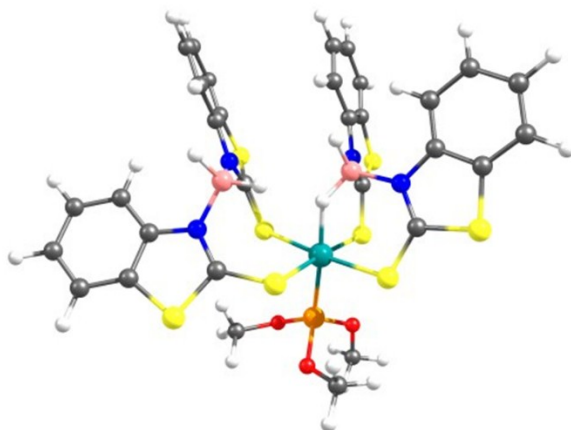
**Fig. 58.** Optimized geometry of **4b**.

T. E. = -4741.44850569 a. u.

Cartesian coordinates for the calculated structure of **4b** (in Å).

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Ru | 0.00034900  | -0.26804600 | -0.53424100 | H | -4.13809200 | -4.80604700 | 3.31750200  |
| P  | -2.07288000 | -0.55029400 | 0.10348500  | C | -3.16400200 | -3.07221600 | 2.49014100  |
| O  | -3.20689500 | 0.63355600  | -0.01794300 | H | -2.26622300 | -3.60157000 | 2.16854900  |
| C  | -3.17766400 | 1.90035400  | 0.54437400  | S | -0.76152700 | 0.14537300  | -2.84420100 |
| C  | -2.55033000 | 2.18410800  | 1.76141100  | S | -0.51501400 | 3.27402500  | -3.13726700 |
| H  | -1.99839200 | 1.40910300  | 2.29298000  | C | -0.47277200 | 1.73749100  | -2.29061400 |
| C  | -2.63756100 | 3.47815900  | 2.28234600  | N | -0.10838800 | 1.83207000  | -1.01270100 |
| H  | -2.14488300 | 3.70214200  | 3.23021800  | C | 0.19313600  | 3.12606300  | -0.63110300 |
| C  | -3.33884100 | 4.47624500  | 1.60551000  | C | 0.63459900  | 3.55546700  | 0.62763000  |
| H  | -3.39966400 | 5.48308800  | 2.02071500  | H | 0.75756900  | 2.82727700  | 1.42924100  |
| C  | -3.95815100 | 4.17735900  | 0.38845600  | C | 0.89491300  | 4.90963800  | 0.82240600  |
| H  | -4.50681900 | 4.95035400  | -0.15259500 | H | 1.24120000  | 5.25207300  | 1.79900200  |
| C  | -3.88080000 | 2.89234000  | -0.14628000 | C | 0.71660900  | 5.84062700  | -0.21266900 |
| H  | -4.36021600 | 2.63757800  | -1.09212700 | H | 0.92699600  | 6.89646400  | -0.03617800 |
| O  | -2.89758800 | -1.70507300 | -0.69131600 | C | 0.27465500  | 5.43092700  | -1.47146200 |
| C  | -4.17369400 | -1.68461000 | -1.26350000 | H | 0.13763000  | 6.15245600  | -2.27803700 |
| C  | -4.40831200 | -0.95907600 | -2.43194700 | C | 0.02013700  | 4.07387900  | -1.67385900 |
| H  | -3.60426000 | -0.35878300 | -2.86121100 | S | 0.25199600  | -2.56242200 | -0.60781300 |
| C  | -5.66792000 | -1.02827100 | -3.02969000 | S | 2.48515200  | -4.49301500 | -0.51075900 |
| H  | -5.85685800 | -0.46330100 | -3.94449500 | C | 4.13931200  | -3.96608400 | -0.66177600 |
| C  | -6.67671200 | -1.81848100 | -2.47241200 | C | 5.29008000  | -4.75269600 | -0.70235200 |
| H  | -7.65769200 | -1.87114000 | -2.94732300 | H | 5.22265700  | -5.83945200 | -0.63944800 |
| C  | -6.42005800 | -2.54572300 | -1.30810200 | C | 6.52515100  | -4.11563200 | -0.82673800 |
| H  | -7.19962000 | -3.16975400 | -0.86729500 | H | 7.43866600  | -4.71076900 | -0.85813800 |
| C  | -5.16648000 | -2.48268500 | -0.69552000 | C | 6.59252300  | -2.71995200 | -0.91093400 |
| H  | -4.95165300 | -3.04420200 | 0.21400700  | H | 7.56246800  | -2.23002600 | -1.00827500 |
| O  | -2.17398400 | -1.05754500 | 1.66569600  | C | 5.44020800  | -1.93397800 | -0.86994200 |
| C  | -3.26500100 | -1.69959400 | 2.25332300  | H | 5.51575100  | -0.85117500 | -0.93091900 |
| C  | -4.39232800 | -0.98005900 | 2.65391300  | C | 4.19382100  | -2.55786000 | -0.74407400 |
| H  | -4.44844000 | 0.09293700  | 2.47050300  | N | 2.93377200  | -1.93821700 | -0.69393300 |
| C  | -5.43663700 | -1.65518100 | 3.29050100  | C | 1.91718300  | -2.83740700 | -0.59233800 |
| H  | -6.32156000 | -1.09778500 | 3.60267200  | S | 0.78837300  | -0.15045600 | 1.67336900  |
| C  | -5.35316700 | -3.02892300 | 3.52897500  | S | 3.25639600  | 0.97057900  | 2.95299800  |
| H  | -6.17195700 | -3.54894300 | 4.02862000  | C | 2.39402700  | 0.35020600  | 1.55801100  |
| C  | -4.21343200 | -3.73330400 | 3.13060500  | N | 3.13516600  | 0.41761100  | 0.41924500  |

|   |            |            |             |   |            |             |             |
|---|------------|------------|-------------|---|------------|-------------|-------------|
| C | 4.34028100 | 1.11250700 | 0.59685000  | C | 5.75456700 | 2.13615700  | 2.31985100  |
| C | 5.24561500 | 1.51558000 | -0.39331600 | H | 5.93717800 | 2.38602800  | 3.36568000  |
| H | 5.03515700 | 1.31065700 | -1.44228800 | C | 4.59548200 | 1.45849100  | 1.94212300  |
| C | 6.39871500 | 2.20534800 | -0.01707100 | B | 2.75545100 | -0.38822200 | -0.86751100 |
| H | 7.10069200 | 2.52409100 | -0.78897800 | H | 3.45348500 | -0.01991100 | -1.78293600 |
| C | 6.66295000 | 2.50240200 | 1.32575500  | H | 1.62218900 | -0.10370100 | -1.33555000 |
| H | 7.57255300 | 3.03904400 | 1.59811200  |   |            |             |             |



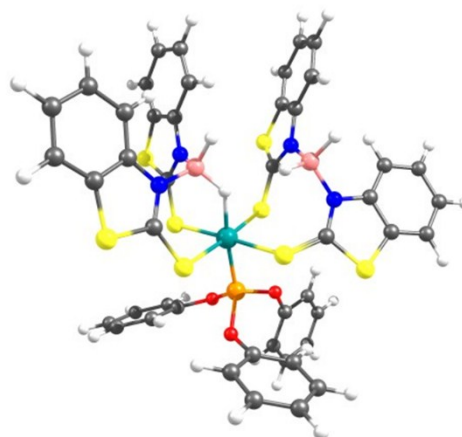
**Fig. 59.** Optimized geometry of **5a**.

T. E. = -5312.53510895 a. u.

Cartesian coordinates for the calculated structure of **5a** (in Å).

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Ru | 0.15229000  | -1.53230200 | 0.23067400  | C | 4.29006600  | 1.21289500  | -1.40275000 |
| P  | 1.23501700  | -3.09184800 | 1.37902800  | C | 5.32711900  | 0.27318000  | -1.59152100 |
| O  | 2.38495800  | -2.67764800 | 2.45237100  | C | 6.66583600  | 0.66510500  | -1.65578000 |
| C  | 3.71163500  | -2.29506100 | 2.04830200  | H | 7.45616700  | -0.07061500 | -1.80992900 |
| H  | 4.19188600  | -3.10493700 | 1.48180500  | C | 6.96447000  | 2.01957200  | -1.51491700 |
| H  | 4.26764500  | -2.10388400 | 2.97447900  | H | 8.00389300  | 2.34847600  | -1.55430700 |
| H  | 3.68639000  | -1.37607600 | 1.44509200  | C | 5.94035100  | 2.95991600  | -1.32571100 |
| O  | 2.08798000  | -4.28118500 | 0.64614100  | H | 6.19236000  | 4.01633800  | -1.22196400 |
| C  | 1.51142000  | -5.10147700 | -0.38335500 | C | 4.60313000  | 2.57245500  | -1.27143500 |
| H  | 0.55801800  | -5.54218500 | -0.05461000 | H | 3.81167600  | 3.30881100  | -1.13777100 |
| H  | 2.23551400  | -5.90360100 | -0.57561500 | B | 1.71685300  | 1.52134000  | -1.62611500 |
| H  | 1.35773300  | -4.52249400 | -1.30444200 | H | 0.83377800  | 0.80478200  | -2.01081300 |
| O  | 0.22755900  | -3.88993000 | 2.36755900  | H | 2.02329800  | 2.34344300  | -2.46023200 |
| C  | 0.71084400  | -4.86151700 | 3.31686300  | N | 1.29956600  | 2.30314200  | -0.31852600 |
| H  | 1.45791200  | -5.52517800 | 2.85819100  | C | 1.20815500  | 1.75746800  | 0.91748400  |
| H  | -0.16330300 | -5.44499200 | 3.63053300  | C | 1.07988000  | 3.68925000  | -0.31916800 |
| H  | 1.15409000  | -4.35454000 | 4.18450400  | C | 0.88861500  | 4.23710900  | 0.97015900  |
| S  | 1.72987400  | -1.80087200 | -1.58956700 | C | 0.68395400  | 5.60429700  | 1.16533400  |
| S  | 4.64394700  | -1.32437700 | -1.70849700 | H | 0.54335200  | 6.00648200  | 2.16938900  |
| S  | 1.36116200  | 0.15840400  | 1.48102600  | C | 0.64943000  | 6.43681700  | 0.04775000  |
| S  | 0.91102600  | 2.96638700  | 2.15526400  | H | 0.48368700  | 7.50733000  | 0.17712900  |
| S  | -1.19895900 | -3.09454700 | -0.86138000 | C | 0.81945500  | 5.90297800  | -1.23734600 |
| S  | -3.88238900 | -3.12582900 | -2.09321800 | H | 0.78377900  | 6.56363100  | -2.10505000 |
| S  | -1.45593200 | -1.43161400 | 1.97892400  | C | 1.03406500  | 4.53939300  | -1.43446700 |
| S  | -3.17214000 | 0.78857200  | 3.03123200  | H | 1.16369800  | 4.13164100  | -2.43493300 |
| C  | 3.02046000  | -0.69216300 | -1.53605200 | C | -2.56850300 | -2.23638900 | -1.34935600 |
| N  | 3.00989800  | 0.65123200  | -1.39917700 | N | -2.81004000 | -0.90150300 | -1.28478900 |

|   |             |             |             |   |             |            |             |
|---|-------------|-------------|-------------|---|-------------|------------|-------------|
| C | -4.04261800 | -0.55096300 | -1.85988400 | N | -2.23003000 | 0.78837400 | 0.61500900  |
| C | -4.77184900 | -1.65134200 | -2.35975100 | C | -2.25595300 | 0.03124600 | 1.74310800  |
| C | -6.01711500 | -1.49531700 | -2.96837300 | C | -2.81106900 | 2.05112700 | 0.79095200  |
| H | -6.56195900 | -2.36003300 | -3.34909800 | C | -3.42348100 | 2.21350300 | 2.05363300  |
| C | -6.54462000 | -0.20838200 | -3.07825100 | C | -4.06975700 | 3.39748600 | 2.40878600  |
| H | -7.51815600 | -0.06277900 | -3.54816200 | H | -4.54335400 | 3.50093100 | 3.38586300  |
| C | -5.82932400 | 0.89135200  | -2.58893200 | C | -4.07809600 | 4.45015800 | 1.49252000  |
| H | -6.24958500 | 1.89401400  | -2.68027100 | H | -4.57078100 | 5.38765500 | 1.75350200  |
| C | -4.58367100 | 0.73420900  | -1.98050600 | C | -3.43873300 | 4.31465700 | 0.25347900  |
| H | -4.04534600 | 1.60109300  | -1.60489100 | H | -3.42405200 | 5.15462200 | -0.44248400 |
| B | -1.79914000 | 0.18305200  | -0.76173200 | C | -2.80415700 | 3.12570100 | -0.10814800 |
| H | -0.60975500 | -0.22603400 | -0.79012200 | H | -2.28990300 | 3.03593300 | -1.06441500 |
| H | -1.73801300 | 1.06903800  | -1.58000400 |   |             |            |             |



**Fig. 60.** Optimized geometry of **5b**.

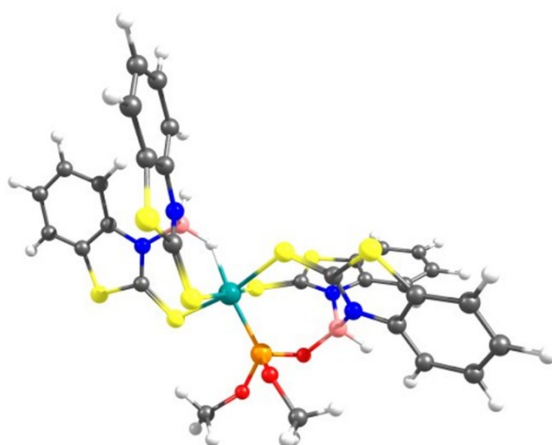
T. E. = -5887.23129634 a. u.

Cartesian coordinates for the calculated structure of **5b** (in Å).

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Ru | -0.31117100 | -0.63368600 | -0.21198100 | C | -2.63584700 | 4.33063000  | -1.81762600 |
| C  | 3.36430600  | 4.49346800  | -0.90442200 | C | -1.58596200 | 2.06593200  | -1.91854900 |
| H  | 3.14939000  | 4.36812100  | -1.96378100 | C | 4.21896000  | -0.11660000 | 0.94713600  |
| C  | 4.39986100  | 5.32192800  | -0.47427100 | C | 5.05199100  | 0.72250700  | 0.19599900  |
| H  | 4.99937400  | 5.84905300  | -1.21816700 | H | 4.73418600  | 1.07257300  | -0.78547200 |
| C  | 4.68327400  | 5.48880500  | 0.88872000  | C | 6.27239800  | 1.12534000  | 0.73859700  |
| H  | 5.49875600  | 6.14281800  | 1.20080300  | H | 6.91665300  | 1.78763100  | 0.15865300  |
| C  | 3.93209000  | 4.81594200  | 1.85110000  | C | 6.67449800  | 0.70602100  | 2.01322800  |
| H  | 4.14871900  | 4.93148900  | 2.91379600  | H | 7.63498500  | 1.02917100  | 2.41672900  |
| C  | 2.90049100  | 3.97814000  | 1.42310900  | C | 5.84206700  | -0.10678700 | 2.78406900  |
| C  | 2.59248400  | 3.81714500  | 0.05243400  | H | 6.13501700  | -0.41729400 | 3.78773900  |
| C  | 1.01278800  | 2.40926800  | 0.94620600  | C | 4.61474900  | -0.49772100 | 2.24832400  |
| C  | -1.26125200 | 4.29466300  | -1.49598700 | C | 2.32728500  | -1.25077500 | 1.60095300  |
| C  | -0.59674700 | 5.48106500  | -1.15707000 | C | 4.94719900  | -2.07787400 | -1.92202500 |
| H  | 0.46565600  | 5.46816900  | -0.91749700 | H | 5.09899100  | -1.11412800 | -1.44210800 |
| C  | -1.31960400 | 6.67147600  | -1.14132300 | C | 6.02920000  | -2.76810400 | -2.46913900 |
| H  | -0.81060200 | 7.59922100  | -0.87576000 | H | 7.02394600  | -2.32422200 | -2.40849500 |
| C  | -2.68569100 | 6.69901500  | -1.46266800 | C | 5.86126400  | -4.01300900 | -3.08768600 |
| H  | -3.22964800 | 7.64444600  | -1.44218800 | H | 6.72178300  | -4.53597900 | -3.50685600 |
| C  | -3.35606700 | 5.52764500  | -1.81033800 | C | 4.59438600  | -4.59102200 | -3.17214800 |
| H  | -4.41631100 | 5.54219400  | -2.06582900 | H | 4.44936000  | -5.55810000 | -3.65508700 |



|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 3.51343000  | -3.89966500 | -2.62566700 | O | -3.19588000 | 0.29749900  | 0.84022200  |
| C | 3.66998000  | -2.64506000 | -1.99805300 | O | -3.35792400 | -2.05607200 | -0.24816100 |
| C | 1.39758400  | -2.89152700 | -1.77614600 | O | -2.52399500 | -1.73889700 | 2.03213100  |
| C | -4.31959800 | 0.49142300  | 1.64177500  | B | 0.86384100  | 2.80025900  | -1.62176100 |
| C | -6.54366100 | 1.10662100  | 3.20712100  | H | 1.30250100  | 3.68641200  | -2.32088600 |
| H | -7.41404600 | 1.34435100  | 3.82047800  | H | 1.09378900  | 1.71500100  | -2.08196900 |
| C | -4.42837700 | 1.75771300  | 2.22255700  | B | 2.40587800  | -0.66305400 | -0.87784400 |
| H | -3.63033900 | 2.48237000  | 2.05595300  | H | 3.04555000  | 0.08843300  | -1.57231800 |
| C | -5.54315700 | 2.06087000  | 3.00360700  | H | 1.26273100  | -0.14649600 | -0.98256600 |
| H | -5.62584200 | 3.04963100  | 3.45851300  | P | -2.32793800 | -1.05246900 | 0.56014400  |
| C | -6.42104400 | -0.15431900 | 2.62084400  | S | -3.18524000 | 2.71904000  | -2.17689000 |
| H | -7.19633400 | -0.90721900 | 2.77436400  | S | 1.85050400  | 2.97684400  | 2.38015800  |
| C | -5.31225300 | -0.47367100 | 1.83241200  | S | 3.34371900  | -1.41410700 | 3.01947400  |
| H | -5.22042700 | -1.45903700 | 1.37853200  | S | 1.83792900  | -4.37662200 | -2.59396000 |
| C | -3.93542400 | -1.90651400 | -1.50921900 | S | 0.72477000  | -1.76470200 | 1.61240500  |
| C | -4.79721600 | -0.84413300 | -1.79204300 | S | -0.23730200 | -2.60054300 | -1.47466700 |
| H | -4.97362100 | -0.06857100 | -1.04804200 | S | -1.36231400 | 0.38861600  | -2.14404800 |
| C | -5.42155700 | -0.78978200 | -3.03899400 | S | -0.27557600 | 1.32976300  | 1.21330100  |
| H | -6.09129200 | 0.04241900  | -3.26348200 | C | -2.24176300 | -3.01601100 | 2.48939500  |
| C | -5.19738500 | -1.78585300 | -3.99200700 | C | -2.29347500 | -3.17667100 | 3.87796600  |
| H | -5.68845800 | -1.73565700 | -4.96491400 | C | -1.94144000 | -4.09645100 | 1.65638900  |
| C | -4.34231400 | -2.84771700 | -3.68999200 | C | -2.03985200 | -4.42836400 | 4.43477800  |
| H | -4.16000300 | -3.63255900 | -4.42620200 | H | -2.52784800 | -2.31236300 | 4.50023600  |
| C | -3.70949000 | -2.91404200 | -2.44773200 | C | -1.68342900 | -5.34342900 | 2.23220100  |
| H | -3.03442300 | -3.73346300 | -2.20047500 | H | -1.90287900 | -3.97003000 | 0.57567000  |
| N | 1.50323200  | 2.96650200  | -0.18617700 | C | -1.73184900 | -5.51854100 | 3.61549400  |
| N | -0.69406100 | 3.02098600  | -1.58142700 | H | -2.08033300 | -4.54993300 | 5.51877700  |
| N | 2.96473700  | -0.62210400 | 0.57930300  |   |             |             |             |
| N | 2.46891300  | -2.09922000 | -1.51511700 |   |             |             |             |



**Fig. 61.** Optimized geometry of **6a**.

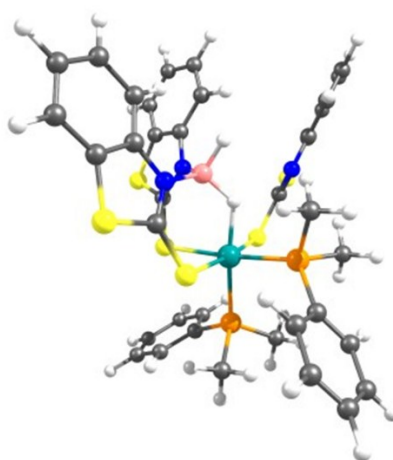
T. E. = -5272.13971484 a. u.

Cartesian coordinates for the calculated structure of **6a** (in Å).

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Ru | 0.37398600  | -0.67407800 | -0.56999500 | S | -0.79711100 | 1.02985000  | 0.61711000  |
| S  | -0.49863200 | -2.46903400 | 0.70904600  | S | -2.81535700 | 3.15114800  | 0.37181100  |
| S  | 1.86705900  | -2.24512600 | -1.45336900 | S | -2.29965900 | -3.00809200 | 2.92566100  |
| P  | -1.20015300 | -1.00075700 | -2.07818500 | S | 4.75969700  | -2.80323500 | -1.30928000 |
| S  | 1.41898200  | 1.05714000  | -1.81399100 | O | -1.46133400 | 0.31226800  | -3.01183300 |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| O | -2.62189900 | -1.44151800 | -1.51482400 | C | 3.36816200  | -1.88526700 | -0.77100800 |
| O | -1.06558400 | -2.21374300 | -3.16395100 | C | -5.41079900 | 3.77516600  | -0.55357100 |
| N | -3.36462000 | 0.73288700  | -0.39425100 | H | -5.30983000 | 4.81285800  | -0.23334300 |
| N | -3.09091600 | -1.44650300 | 1.01164200  | C | -6.56322600 | 3.33447900  | -1.20391400 |
| C | 3.36479400  | 2.43004300  | 1.30178700  | H | -7.37806700 | 4.03481400  | -1.39188300 |
| C | -3.89043900 | -2.32094500 | 3.05616300  | C | -4.37947100 | 2.86068000  | -0.33376000 |
| C | -2.35850300 | 1.46962700  | 0.14815900  | C | -6.67073600 | 2.00295400  | -1.62557800 |
| N | 3.67742400  | -0.98474300 | 0.19973300  | H | -7.57080400 | 1.67193200  | -2.14578200 |
| C | -4.48645200 | 1.50841500  | -0.73035200 | C | 7.77399700  | -1.39994300 | 1.03681400  |
| C | -5.64526200 | 1.08458000  | -1.39801400 | H | 8.83938800  | -1.53232800 | 1.22943200  |
| H | -5.73850000 | 0.05233500  | -1.73070200 | B | 2.64387200  | -0.07042700 | 0.95304000  |
| C | -4.13836400 | -1.47906500 | 1.95122700  | C | -6.28982200 | -0.95889500 | 2.90589000  |
| C | -2.02184600 | -2.18495500 | 1.40049900  | H | -7.23542300 | -0.41731700 | 2.85286200  |
| C | 5.78532200  | -1.98021800 | -0.16659700 | C | 7.03937600  | -0.45902000 | 1.76865400  |
| B | -3.41066300 | -0.85832300 | -0.43879000 | H | 7.53705000  | 0.14063900  | 2.53218500  |
| C | -6.03651600 | -1.80802700 | 3.99048700  | S | 3.02382800  | 3.46583100  | -1.05420400 |
| H | -6.78233500 | -1.92704000 | 4.77761100  | N | 2.74675400  | 1.43242300  | 0.53414500  |
| C | -4.82903800 | -2.50009800 | 4.07340700  | C | 2.40472600  | 1.86174400  | -0.71117000 |
| H | -4.61657400 | -3.16058800 | 4.91489500  | C | 4.60774700  | 4.63161100  | 2.51294400  |
| C | -5.35548700 | -0.78679800 | 1.88436700  | H | 5.09505000  | 5.48064200  | 2.99391100  |
| H | -5.57695600 | -0.12209300 | 1.05233500  | C | 4.27053900  | 4.70499900  | 1.16083900  |
| C | -0.11925400 | -2.09230000 | -4.23996700 | H | 4.48015700  | 5.60334900  | 0.57892000  |
| H | 0.84997100  | -1.70456700 | -3.89317700 | C | 4.30216900  | 3.48448400  | 3.25609500  |
| H | -0.51314900 | -1.43260500 | -5.02860900 | H | 4.54374400  | 3.44955400  | 4.31945800  |
| H | 0.02226500  | -3.10231700 | -4.64358300 | C | 3.63963200  | 3.60842000  | 0.57324800  |
| C | -2.55587900 | 0.34252000  | -3.94942200 | C | 3.68183800  | 2.38280400  | 2.66574700  |
| H | -2.76252800 | -0.65466600 | -4.36478100 | H | 3.42507000  | 1.50397300  | 3.25608000  |
| H | -2.26434800 | 1.02882800  | -4.75482500 | H | -4.56547800 | -1.16122300 | -0.62561300 |
| H | -3.46264100 | 0.72136900  | -3.45659000 | H | 1.48032300  | -0.54148800 | 0.88629500  |
| C | 5.67623600  | -0.26665400 | 1.54164000  | H | 2.84778600  | -0.16503100 | 2.14042700  |
| H | 5.12474400  | 0.47168000  | 2.11867900  |   |             |             |             |
| C | 5.03423200  | -1.03272100 | 0.56200700  |   |             |             |             |
| C | 7.14800800  | -2.17316700 | 0.05899200  |   |             |             |             |
| H | 7.70694200  | -2.91309900 | -0.51514700 |   |             |             |             |





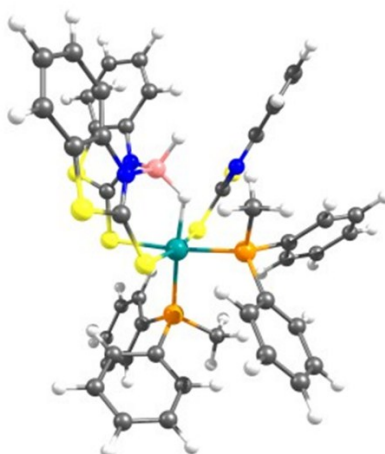
**Fig. 62.** Optimized geometry of **7a**.

T. E. = -4785.13330884 a. u.

Cartesian coordinates for the calculated structure of **7a** (in Å).

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Ru | 1.12567600  | -0.10886900 | 0.08687700  | H | 4.06629900  | 1.48867200  | 3.05999700  |
| P  | 1.78108200  | -1.07574700 | -1.91519900 | C | 3.46843600  | 0.86402600  | 5.02702100  |
| C  | 0.75360300  | -0.49334300 | -3.32747500 | H | 3.90105800  | 1.74484400  | 5.50539500  |
| H  | 1.09354300  | -0.94405200 | -4.27024700 | C | 2.82509300  | -0.10686400 | 5.79553600  |
| H  | 0.80638600  | 0.60036700  | -3.40321300 | H | 2.75325800  | 0.00922300  | 6.87849800  |
| H  | -0.28290000 | -0.78924000 | -3.11551500 | C | 2.26555600  | -1.22357100 | 5.16979900  |
| C  | 1.61598800  | -2.89409200 | -2.10273300 | H | 1.74920600  | -1.98235000 | 5.76071000  |
| H  | 0.54604200  | -3.11728200 | -2.00518900 | C | 2.35323900  | -1.37132100 | 3.78560200  |
| H  | 2.14786700  | -3.42737900 | -1.30618800 | H | 1.88474900  | -2.23527300 | 3.31038500  |
| H  | 1.97644700  | -3.22032300 | -3.08836100 | S | 0.18101400  | -2.16027700 | 0.94301700  |
| C  | 3.48259000  | -0.76280400 | -2.56944600 | S | -2.18040400 | -3.98356400 | 0.74725800  |
| C  | 4.45229100  | -1.77679200 | -2.64164700 | S | 1.88328700  | 2.02013900  | -0.54411300 |
| H  | 4.20630300  | -2.79566200 | -2.33836400 | S | 0.61554200  | 4.64095600  | -1.11237200 |
| C  | 5.74014400  | -1.50871500 | -3.11422700 | S | 0.24049500  | 0.92722100  | 2.13337700  |
| H  | 6.47598600  | -2.31398400 | -3.16064700 | S | -2.55836700 | 1.00216800  | 3.21386500  |
| C  | 6.08128200  | -0.22182600 | -3.53250300 | C | -1.16678200 | -2.70103300 | 0.01213800  |
| H  | 7.08590600  | -0.01214200 | -3.90393500 | N | -1.56931700 | -2.31522900 | -1.17807100 |
| C  | 5.12349100  | 0.79415200  | -3.47784900 | C | -2.69820900 | -2.99937100 | -1.58340400 |
| H  | 5.37620500  | 1.80368100  | -3.80785800 | C | -3.36892800 | -2.80872500 | -2.80261400 |
| C  | 3.83976500  | 0.52754600  | -3.00017700 | H | -2.99234000 | -2.06702600 | -3.50953200 |
| H  | 3.11245900  | 1.33858600  | -2.94402200 | C | -4.50002900 | -3.57150000 | -3.08937900 |
| P  | 3.07903700  | -0.61463300 | 1.17455400  | H | -5.02149500 | -3.42581200 | -4.03727400 |
| C  | 3.72715800  | -2.33323200 | 1.04046800  | C | -4.97584800 | -4.52686000 | -2.17794900 |
| H  | 2.93129700  | -3.05352000 | 1.26899600  | H | -5.86224300 | -5.11530200 | -2.42072400 |
| H  | 4.07278100  | -2.50264800 | 0.01258700  | C | -4.32484000 | -4.73643400 | -0.95973000 |
| H  | 4.56972700  | -2.47651200 | 1.73081900  | H | -4.69588300 | -5.48010100 | -0.25279900 |
| C  | 4.57503400  | 0.35416000  | 0.71912300  | C | -3.19327100 | -3.97182400 | -0.66912300 |
| H  | 4.36754500  | 1.43035000  | 0.77432900  | C | -1.42326200 | 0.90779800  | 1.88623600  |
| H  | 5.41425000  | 0.10411800  | 1.38290000  | N | -2.04293700 | 0.75300200  | 0.69029600  |
| H  | 4.84648400  | 0.11496000  | -0.31704400 | C | -3.42568800 | 0.56420700  | 0.80679400  |
| C  | 3.01538500  | -0.40896400 | 3.00462600  | C | -4.32769900 | 0.22064200  | -0.20812400 |
| C  | 3.56272900  | 0.71502700  | 3.64125500  | H | -3.96874700 | 0.03655600  | -1.21980500 |

|   |             |             |             |   |             |            |             |
|---|-------------|-------------|-------------|---|-------------|------------|-------------|
| C | -5.67827000 | 0.07904000  | 0.11067000  | C | -3.85123800 | 4.52751900 | -1.57896300 |
| H | -6.38008600 | -0.20258900 | -0.67551800 | H | -4.93373600 | 4.43562500 | -1.67892400 |
| C | -6.14169000 | 0.27208900  | 1.41885200  | C | -3.23941600 | 5.77200400 | -1.77310800 |
| H | -7.20244100 | 0.15555200  | 1.64465100  | H | -3.84343200 | 6.64523100 | -2.02298900 |
| C | -5.24999200 | 0.58707200  | 2.44455200  | C | -1.85593100 | 5.90317800 | -1.64803400 |
| H | -5.59726900 | 0.71212500  | 3.47084500  | H | -1.36702100 | 6.86618200 | -1.80036000 |
| C | -3.89720300 | 0.71632100  | 2.12955000  | C | -1.11012200 | 4.77001500 | -1.32445000 |
| C | 0.47895600  | 2.92461300  | -0.78543200 | B | -1.27129200 | 0.99178400 | -0.64305100 |
| N | -0.80643500 | 2.48874400  | -0.80677200 | H | -0.35930600 | 0.13894500 | -0.87124800 |
| C | -1.71592800 | 3.51090000  | -1.12280700 | H | -1.99574200 | 0.72958100 | -1.57315400 |
| C | -3.10485200 | 3.39432800  | -1.25421100 |   |             |            |             |
| H | -3.59974400 | 2.43753900  | -1.10254000 |   |             |            |             |



**Fig. 63.** Optimized geometry of **7b**.

T. E. = -5168.23266024 a. u.

Cartesian coordinates for the calculated structure of **7b** (in Å).

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Ru | -0.69116300 | -0.12771100 | 0.20721000  | H | -4.42065300 | 1.68084000  | 2.01685000  |
| P  | -1.09273400 | 1.50062200  | -1.45531700 | C | -2.79037300 | -0.40683400 | 3.12731900  |
| C  | -0.10220800 | 1.05662900  | -2.94539600 | C | -3.97984700 | -0.91064900 | 3.68084100  |
| H  | -0.38840700 | 1.64740100  | -3.82422200 | H | -4.84087400 | -1.10759900 | 3.04111900  |
| H  | -0.26830100 | -0.00592800 | -3.16164100 | C | -4.07660300 | -1.16794700 | 5.04957600  |
| H  | 0.95612300  | 1.21081500  | -2.69760200 | H | -5.00866400 | -1.56339900 | 5.45828300  |
| C  | -2.78377400 | 1.64388900  | -2.21528700 | C | -2.98919200 | -0.92041100 | 5.89006000  |
| C  | -3.58413300 | 2.78442300  | -2.03592600 | H | -3.06436300 | -1.12366400 | 6.96007500  |
| H  | -3.21146000 | 3.62382900  | -1.44675400 | C | -1.80672300 | -0.41148400 | 5.35183700  |
| C  | -4.84575700 | 2.87594300  | -2.62989000 | H | -0.94952800 | -0.21201800 | 5.99770500  |
| H  | -5.44709300 | 3.77471700  | -2.47847500 | C | -1.70536000 | -0.15819700 | 3.98177600  |
| C  | -5.32602400 | 1.83526500  | -3.42684200 | H | -0.76984100 | 0.23608000  | 3.58355300  |
| H  | -6.30640400 | 1.91159800  | -3.90095800 | S | 0.39834400  | 1.38441300  | 1.73776700  |
| C  | -4.53618200 | 0.69995300  | -3.61989300 | S | 2.76608800  | 3.17668100  | 2.05518000  |
| H  | -4.89821400 | -0.12149500 | -4.24120000 | S | -1.51272900 | -1.81104900 | -1.22230800 |
| C  | -3.28091400 | 0.60189800  | -3.01750600 | S | -0.34559300 | -4.09555100 | -2.70628000 |
| H  | -2.68848800 | -0.30126200 | -3.16896100 | S | -0.06380400 | -1.91585800 | 1.73460100  |
| P  | -2.70249400 | 0.08122400  | 1.33382300  | S | 2.61799900  | -2.67113800 | 2.86317500  |
| C  | -3.45004800 | 1.75521500  | 1.50810400  | C | 1.75435100  | 2.15051000  | 0.99085700  |
| H  | -2.76958200 | 2.35180900  | 2.12920900  | N | 2.16250600  | 2.09719900  | -0.25356500 |
| H  | -3.57248000 | 2.24309600  | 0.53436900  | C | 3.29908600  | 2.85437400  | -0.45097400 |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 3.98066400  | 2.99495700  | -1.67105100 | C | 2.08876800  | -5.26210800 | -3.54577100 |
| H | 3.60262900  | 2.48118100  | -2.55681900 | H | 1.56177900  | -6.04649900 | -4.09040100 |
| C | 5.12399000  | 3.79053300  | -1.73009800 | C | 1.38231000  | -4.28209800 | -2.84902100 |
| H | 5.65345900  | 3.90272700  | -2.67817400 | B | 1.68827800  | -1.07776600 | -0.75646500 |
| C | 5.60276200  | 4.45171200  | -0.58843200 | H | 0.83594900  | -0.13333100 | -0.70155900 |
| H | 6.49887100  | 5.07100800  | -0.65502100 | H | 2.50190800  | -0.54420100 | -1.46956100 |
| C | 4.94255100  | 4.32803300  | 0.63672500  | C | -4.08141300 | -0.91440800 | 0.62373900  |
| H | 5.31630100  | 4.84311200  | 1.52300900  | C | -5.15061000 | -0.32951400 | -0.06872100 |
| C | 3.79724200  | 3.53225300  | 0.69817400  | C | -4.04045200 | -2.31501400 | 0.74594200  |
| C | 1.61592900  | -1.96449500 | 1.61591200  | C | -6.16493800 | -1.12406100 | -0.61115600 |
| N | 2.34740600  | -1.42057500 | 0.61411200  | H | -5.20126700 | 0.75217300  | -0.19853200 |
| C | 3.72242600  | -1.41519800 | 0.87720600  | C | -5.05738300 | -3.10504500 | 0.21239300  |
| C | 4.72808100  | -0.78555900 | 0.13313700  | H | -3.21135500 | -2.79106100 | 1.27363600  |
| H | 4.47002200  | -0.19048700 | -0.74204200 | C | -6.12472800 | -2.51108500 | -0.46747300 |
| C | 6.05088100  | -0.90051400 | 0.55966900  | H | -6.98914500 | -0.65012100 | -1.14757200 |
| H | 6.83531700  | -0.39981900 | -0.00955200 | H | -5.01305700 | -4.18998400 | 0.32395500  |
| C | 6.38430200  | -1.62684700 | 1.71103500  | H | -6.92041700 | -3.12993100 | -0.88648800 |
| H | 7.42606200  | -1.70234300 | 2.02535200  | C | -0.69006200 | 3.29073400  | -1.22484600 |
| C | 5.38886000  | -2.23419800 | 2.47706600  | C | -0.16118700 | 4.06130800  | -2.27355500 |
| H | 5.63654800  | -2.77810000 | 3.38937200  | C | -0.95778200 | 3.92511800  | -0.00269400 |
| C | 4.06389900  | -2.10962900 | 2.05860800  | C | 0.09283500  | 5.42259000  | -2.10303900 |
| C | -0.14167700 | -2.65671500 | -1.72475600 | H | 0.06639400  | 3.60627800  | -3.23680700 |
| N | 1.16375800  | -2.35904600 | -1.50206400 | C | -0.70803000 | 5.28914400  | 0.16671000  |
| C | 2.03871700  | -3.25509200 | -2.13683800 | H | -1.32489300 | 3.34029900  | 0.83746700  |
| C | 3.43799000  | -3.21509200 | -2.13139700 | C | -0.18220000 | 6.04318000  | -0.88255200 |
| H | 3.97047600  | -2.43582800 | -1.59017700 | H | 0.51303300  | 5.99900200  | -2.92940200 |
| C | 4.14490200  | -4.19482700 | -2.82949300 | H | -0.91402600 | 5.75777200  | 1.13088900  |
| H | 5.23541400  | -4.16384300 | -2.82389900 | H | 0.02240700  | 7.10692900  | -0.74838000 |
| C | 3.48319100  | -5.21125700 | -3.52931300 |   |             |             |             |
| H | 4.05664400  | -5.96864600 | -4.06530300 |   |             |             |             |