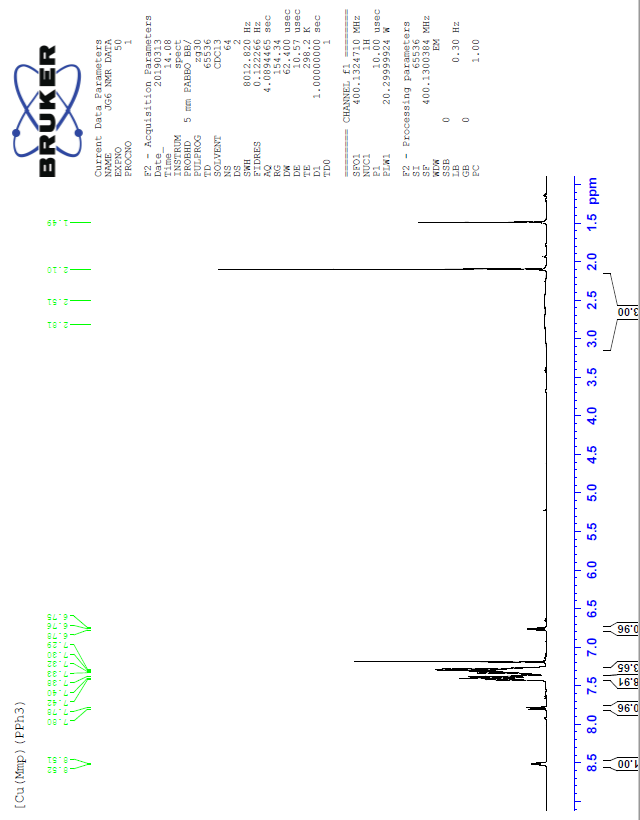
**Supplementary Materials: Adding to the Family of Copper Complexes Featuring Borohydride Ligands Based on 2-Mercaptopyridyl Units**

Joseph Goldsworthy, Simon D. Thomas, Graham J. Tizzard, Simon J. Coles and Gareth R. Owen

**Table S1.** Crystallographic Parameters for the two complexes.

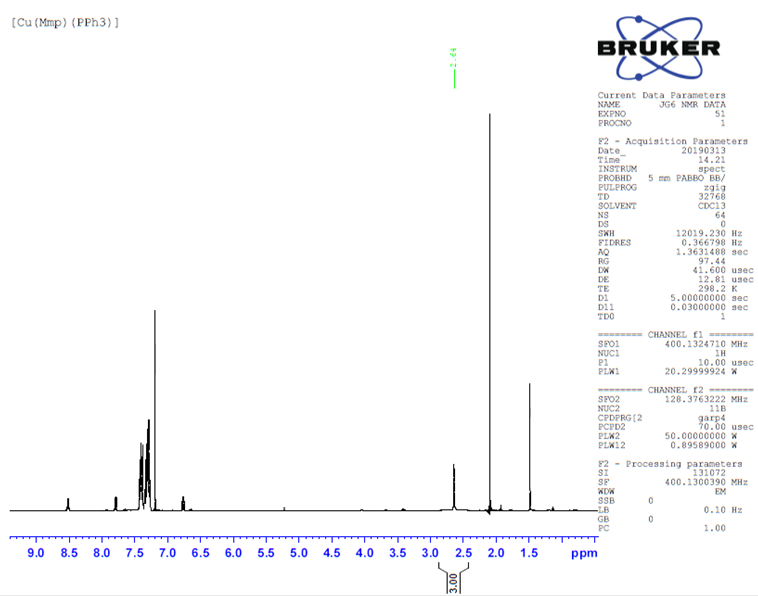
|  |  |  |
| --- | --- | --- |
| **Complex** | **1** | **2** |
| Formula | C23H22BCuNPS | C23H40BCuNPS |
| *Dcalc.*/ g cm-3 | 1.427 | 1.296 |
| **/mm-1 | 3.175 | 2.773 |
| Formula Weight | 449.79 | 467.94 |
| Colour | light yellow | colourless |
| Shape | block | block |
| Size/mm3 | 0.13×0.09×0.07 | 0.18×0.12×0.04 |
| *T*/K | 100(2) | 100(2) |
| Crystal System | monoclinic | triclinic |
| Space Group | *C*2/*c* | *P*-1 |
| *a*/Å | 11.90994(6) | 8.16720(10) |
| *b*/Å | 13.21619(7) | 9.38370(10) |
| *c*/Å | 26.83905(13) | 17.2612(2) |
| **/° | 90 | 96.9390(10) |
| **/° | 97.6274(4) | 95.6170(10) |
| **/° | 90 | 112.3730(10) |
| V/Å3 | 4187.20(4) | 1199.33(3) |
| *Z* | 8 | 2 |
| *Z'* | 1 | 1 |
| Wavelength/Å | 1.54178 | 1.54178 |
| Radiation type | Cu K** | Cu K** |
| *min*/° | 3.323 | 2.611 |
| *max*/° | 70.065 | 70.033 |
| Measured Refl. | 38239 | 30937 |
| Independent Refl. | 3963 | 4471 |
| Reflections with I > 2(I) | 3908 | 4402 |
| *Rint* | 0.0259 | 0.0278 |
| Parameters | 290 | 285 |
| Restraints | 68 | 37 |
| Largest Peak | 0.316 | 0.330 |
| Deepest Hole | −0.349 | −0.364 |
| GooF | 1.065 | 1.052 |
| *wR2* (all data) | 0.0661 | 0.0628 |
| *wR2* | 0.0659 | 0.0625 |
| *R1* (all data) | 0.0246 | 0.0239 |
| *R1* | 0.0244 | 0.0236 |



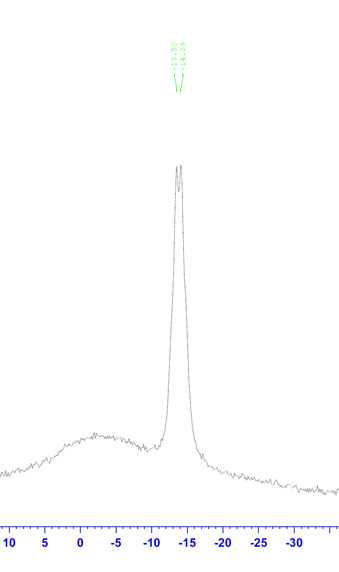
acetone

H2O

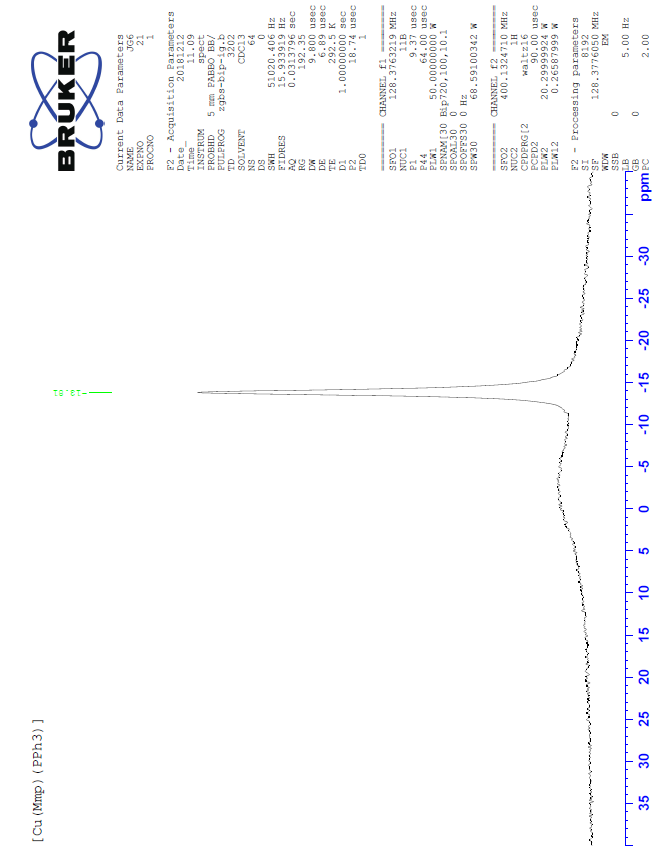
**Figure S1.** 1H NMR (CDCl3) of [Cu{H3B(mp)}(PPh3)].



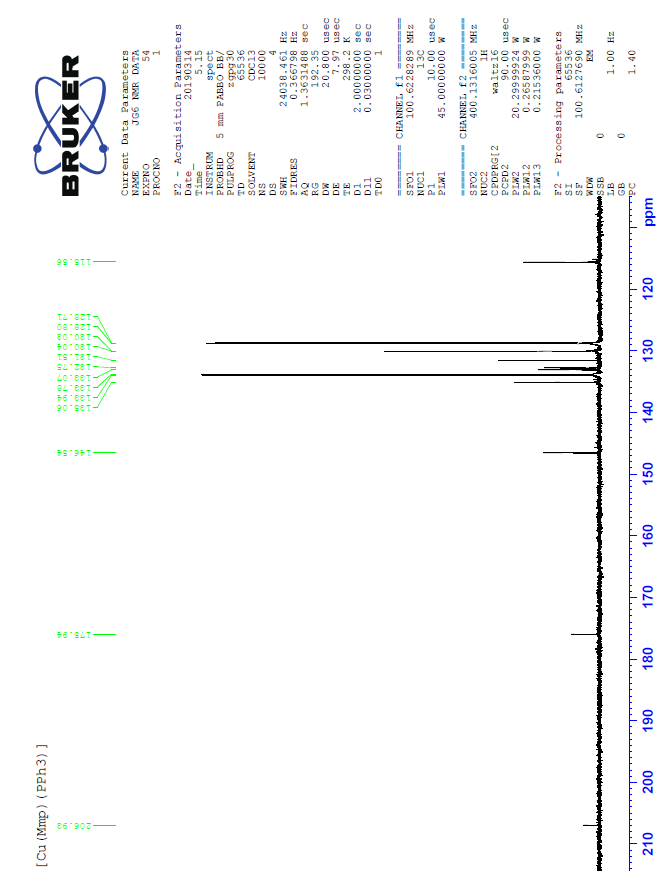
**Figure S2.** 1H{11B} NMR (CDCl3) of [Cu{H3B(mp)}(PPh3)] with a particular focus on BH3-.



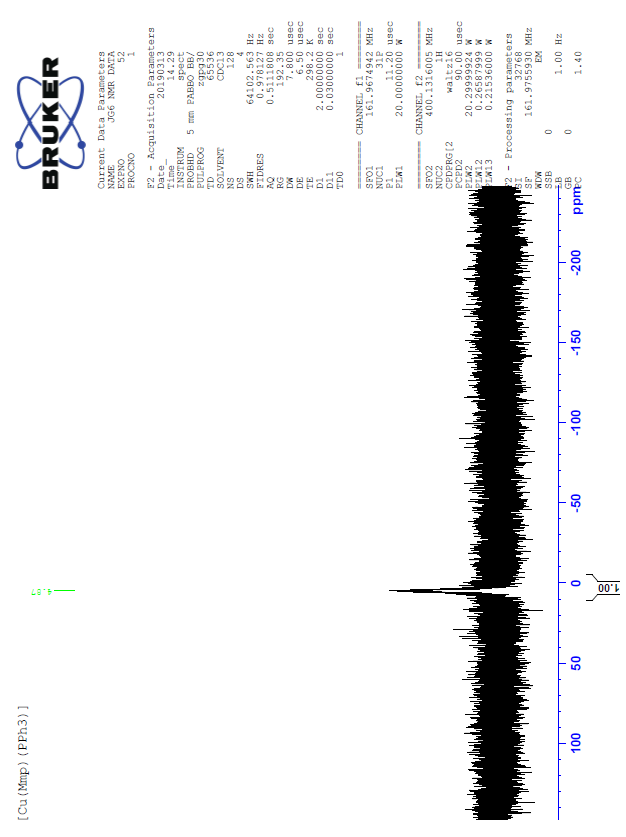
**Figure S3.** 11B NMR (CDCl3) of [Cu{H3B(mp)}(PPh3)].



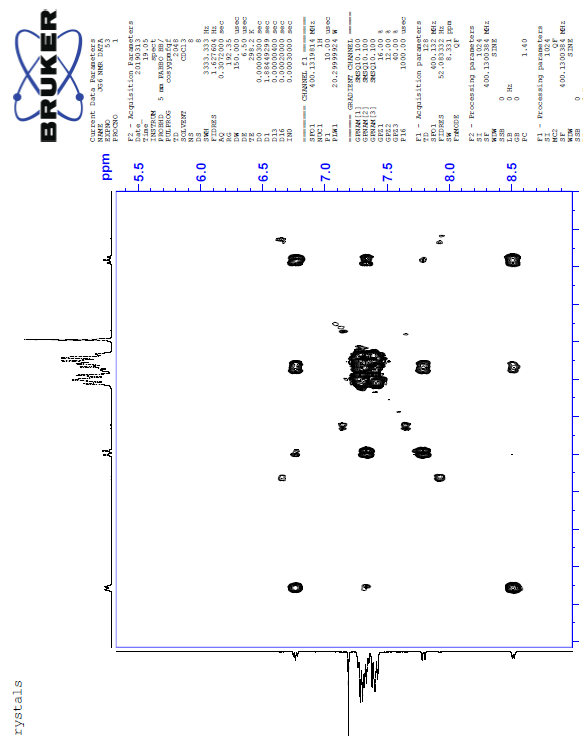
**Figure S4.** 11B{1H} NMR (CDCl3) of [Cu{H3B(mp)}(PPh3)].



**Figure S5.** 13C{1H} NMR (CDCl3) of [Cu{H3B(mp)}(PPh3).

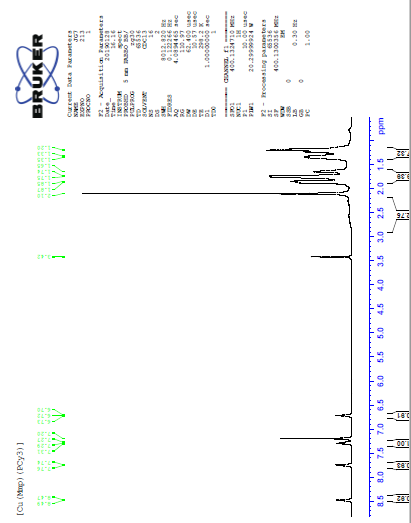


**Figure S6.** 31P{1H} NMR (CDCl3) of [Cu{H3B(mp)}(PPh3).

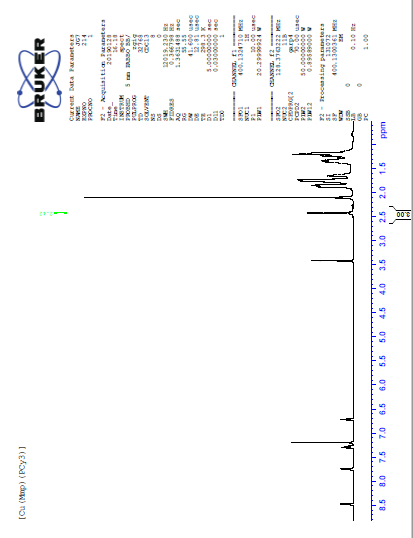


mpCH-(5)

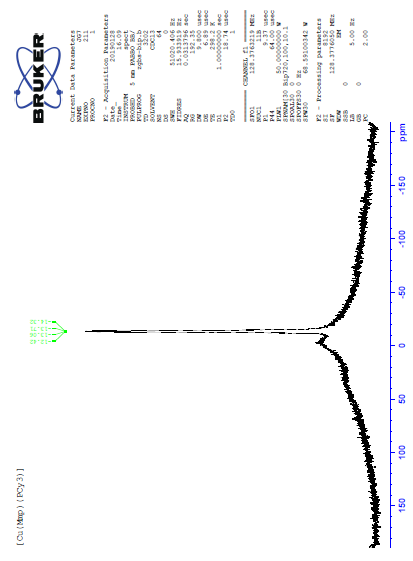
**Figure S7.** COSY NMR (CDCl3) of [Cu{H3B(mp)}(PPh3)].



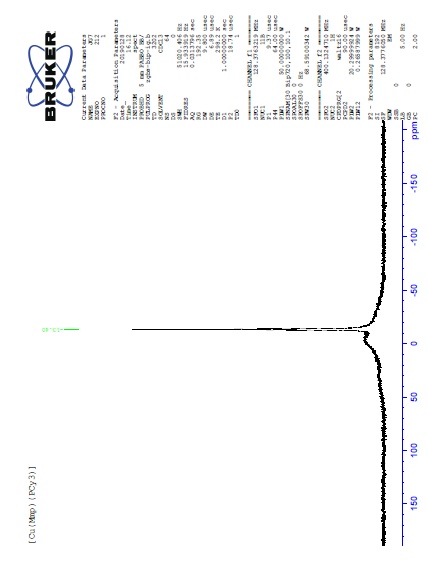
**Figure S8.** 1H NMR (CDCl3) of [Cu{H3B(mp)}(PCy3)].



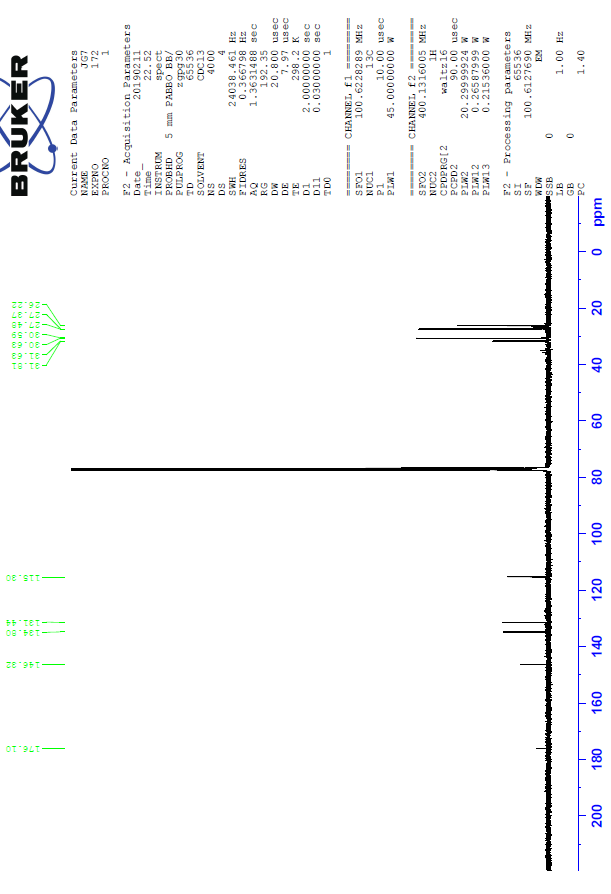
**Figure S9.** 1H{11B} NMR (CDCl3) of [Cu{H3B(mp)}(PCy3)] with a particular focus on BH3- unit.



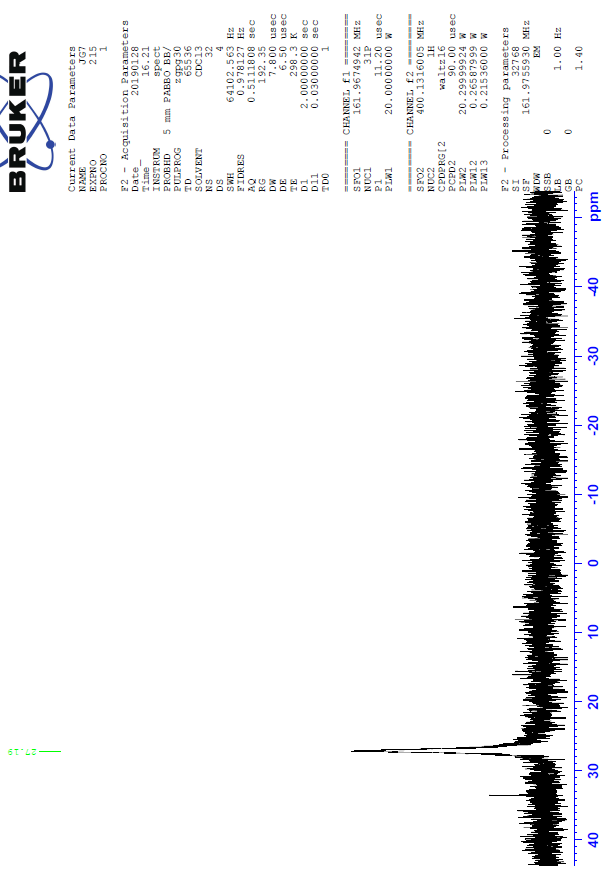
**Figure S10.** 11B NMR (CDCl3) of [Cu{H3B(mp)}(PCy3)].



**Figure S11.** 11B{1H} NMR (CDCl3) of [Cu{H3B(mp)}(PCy3)].



**Figure S12.** 13C{1H} NMR (CDCl3) of [Cu{H3B(mp)}(PCy3)].



**Figure S13.** 31P{1H} NMR (CDCl3) of [Cu{H3B(mp)}(PCy3)].