Supporting Information for B911439D

Unprecedented cubane-type silver cluster with a novel phosphinite-functionalized N-heterocyclic carbene ligand

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- Crystal structure determination of 4 (Fig. S-1)
- NMR spectra of compounds 1-4.

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Crystal structure determination of 4.

The two independent molecules show a very similar structure. Their overlapped structures (blue and red spheres) are shown below (Fig. S-1).

Fig. S-1. View of the overlapped structures of the two independent molecules of 4 which show a very similar structure.
NMR spectra of compounds 1-4.

**Compound 1 \(^1\text{H} \text{NMR, } d_6\text{-DMSO}**
Compound 1 $^{13}$C\textsuperscript{1}H NMR, $d_6$-DMSO
Compound 2 $^1$H NMR, $d_6$-DMSO
Compound 2 $^{13}$C($^1$H) NMR, $d_6$-DMSO
Compound 3 $^{31}\text{P}\{^1\text{H}\}$ NMR, CDCl$_3$
Compound 3 $^1$H NMR, CDCl$_3$
Compound 3 \(^{13}\text{C}\{^1\text{H}\}\) NMR, CDCl\(_3\)
Compound 4 $^{31}\text{P}^1\text{H}$ NMR, CD$_2$Cl$_2$
Compound 4 $^1$H NMR, CD$_2$Cl$_2$
Compound 4 $^{13}$C-$^1$H NMR, CD$_2$Cl$_2$