Supporting Information for

“Dicopper-[18]ane-N₆ Complexes: Structures, Magnetism and Phosphate Monoester Binding”

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Figure S1. Spectroscopic titration of compound 1 by hydrogen phosphate.

Figure S2. Changes of optical density (o) of a 1.0 mM solution of 1 titrated with HPO$_4^{2-}$, monitored at 640 nm. Theoretical fit shown as the solid line up to 1.4 molar equiv.
Figure S3. Spectroscopic titration of compound 1 by phenyl phosphate.

Figure S4. Changes of optical density (o) of a 1.0 mM solution of 1 titrated with phenyl phosphate, monitored at 640 nm. Theoretical fit is shown as the solid line.
**Figure S5.** Spectroscopic titration of compound 1 by DL-α-glycerol phosphate

**Figure S6.** Changes of optical density (o) of a 1.0 mM solution of 1 titrated with DL-α-glycerol phosphate, monitored at 640 nm. Theoretical fit shown as solid line.
**Figure S7.** Spectroscopic titration of compound 1 by α-D-glucose phosphate

**Figure S8.** Changes of optical density (o) of a 1.0 mM solution of 1 buffered to a pH of 7.4 with 5mM HEPES being titrated with α-D-glucose phosphate, monitored at 640 nm. Theoretical fit is shown as the solid line.
**Figure S9.** Spectroscopic titration of 1 by $\text{HPO}_4^{2-}$ buffered with 5 mM HEPES at pH=7.4.

**Figure S10.** Changes of optical density (o) of a 1.0 mM solution of 1 buffered to a pH of 7.4 with 5mM HEPES being titrated with $\text{HPO}_4^{2-}$, monitored at 640 nm. Theoretical fit is shown as the solid line.

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<th>$y = a + b\times\lambda$</th>
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<td>Value</td>
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Figure S11. Spectroscopic titration of compound 1 by phenyl phosphate buffered with 5 mM HEPES at pH = 7.4.

Figure S12. Changes of optical density (o) of a 1.0 mM solution of 1 buffered to a pH of 7.4 with 5mM HEPES titrated with phenyl phosphate, monitored at 640 nm. Theoretical fit is shown as the solid line.
Figure S13. Spectroscopic titration of compound 1 by β-glycerol phosphate buffered with 5 mM HEPES at pH = 7.4.

Figure S14. Changes of optical density (o) of a 1.0 mM solution of 1 buffered to a pH of 7.4 with 5 mM HEPES titrated with β-glycerol phosphate, monitored at 640 nm. Theoretical fit is shown as the solid line.
**Figure S15.** Spectroscopic titration of compound 1 by DL-α-glycerol phosphate buffered with 5 mM HEPES at pH = 7.4.

**Figure S16.** Changes of optical density (o) of a 1.0 mM solution of 1 buffered to a pH of 7.4 with 5mM HEPES being titrated with DL-α-glycerol phosphate, monitored at 640 nm. Theoretical fit is shown as the solid line.
Figure S17. Spectroscopic titration of compound 1 by α-D-glucose phosphate buffered with 5 mM HEPES at pH = 7.4.

Figure S18. Changes of optical density (o) of a 1.0 mM solution of 1 buffered to a pH of 7.4 with 5mM HEPES being titrated with (C₆H₁₁O₆)PO₃⁻, monitored at 640 nm. Theoretical fit is shown as the solid line.
Figure S19. Spectroscopic titration of compound 1 with 40 equivalents of HEPES.

Figure S20. Changes of optical density (o) of a 1.0 mM solution of 1 titrated with a HEPES solution adjusted to a pH of 7.4, monitored at 640 nm. Theoretical fit is shown as the solid line.