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1:2 Adducts of copper(I) halides with 1,2-bis(di-2-pyridylphosphino)ethane: Solid state and solution structural studies and antitumour activity

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Supplementary Information

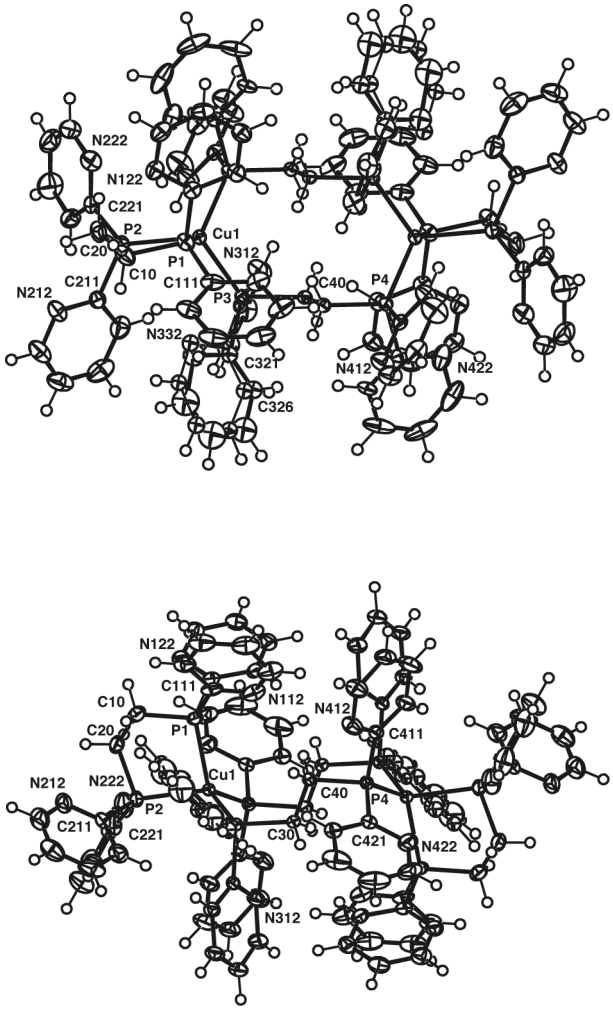

Fig. S1 Molecular structure of the cation of (**2**, X=Br) showing the numbering scheme. Ellipsoids are plotted at the 50% level.

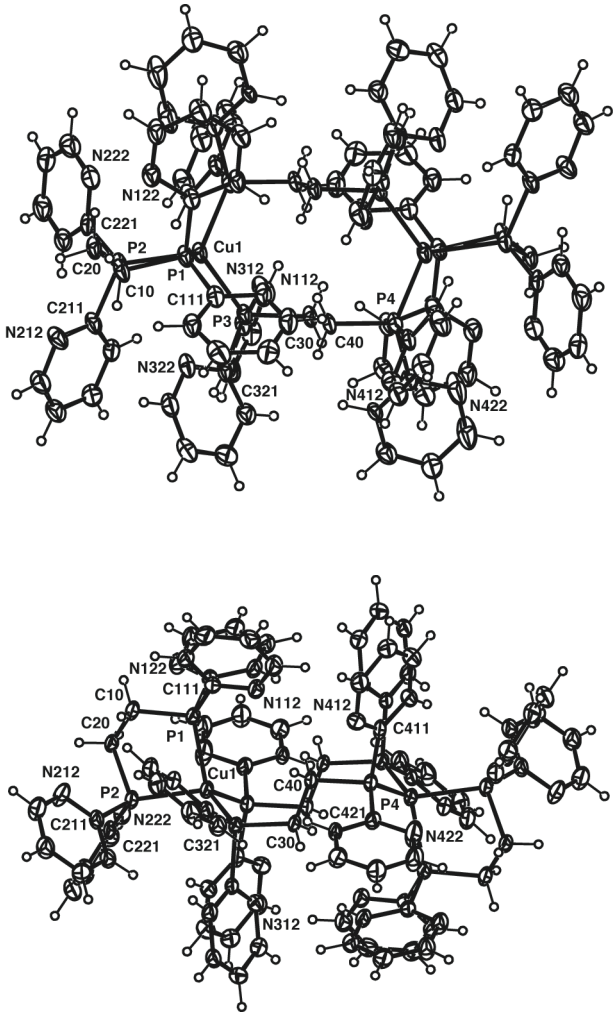

Fig. S2 Molecular structure of the cation of (**3** X=I**)** showing the numbering scheme. Ellipsoids are plotted at the 50% level.

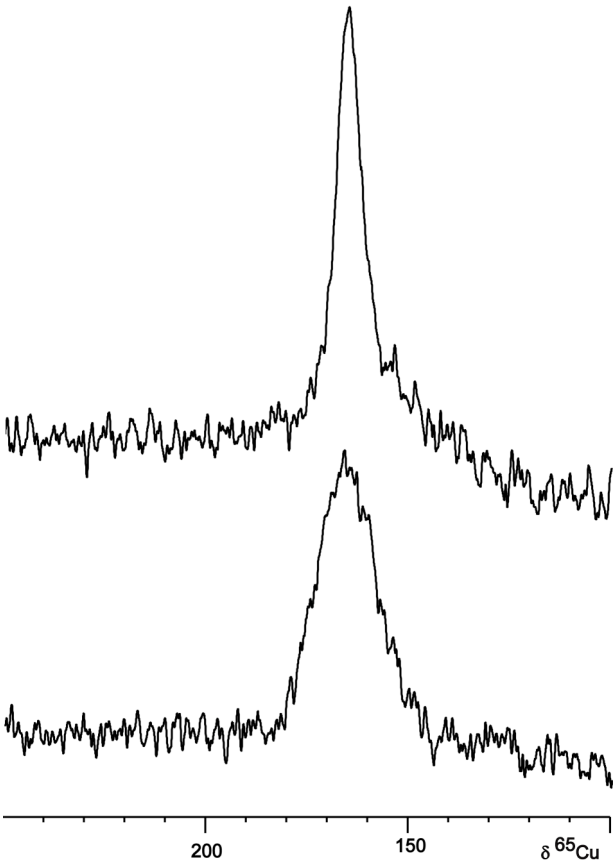

Fig S3. ^{65}Cu NMR spectra of a 61 mM solution of [Cu(d2pype)$_2$]Cl in MeOD at 333 K recorded with (top, $\Delta\nu_{1/2}$ = 1324.0 Hz) and without (bottom, $\Delta\nu_{1/2}$ = 2648.9 Hz) ^{31}P-decoupling.

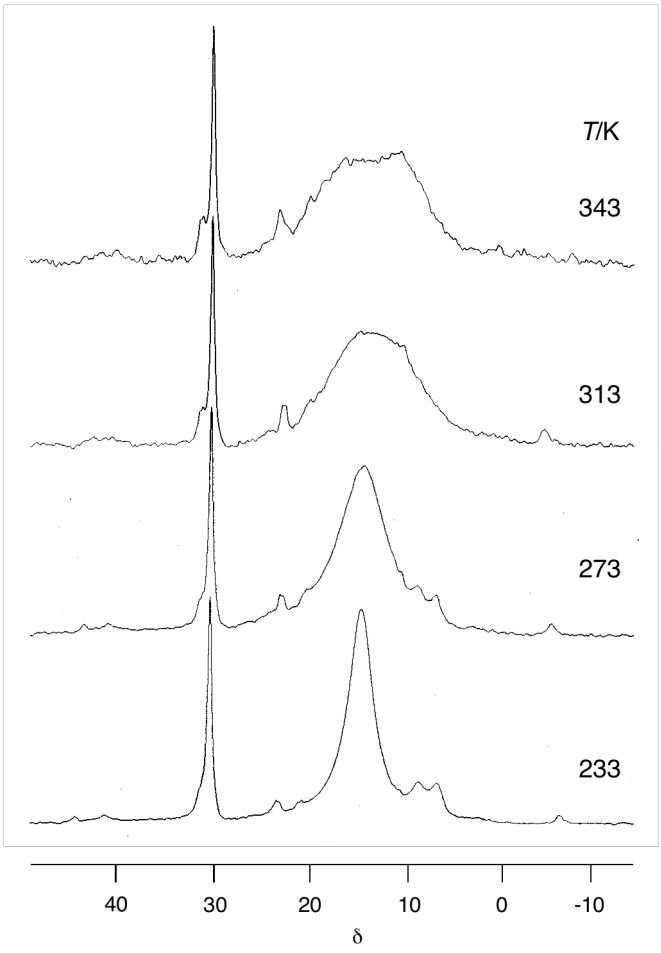

Fig S4. 161.9 MHz $^{31}P\{^{1}H\}$ NMR spectra of a solution of $\{[Cu(d2pype)_2]I\}_n$ in $CDCl_3$ at the temperatures indicated. The lineshape of the resonance at δ 13.9 over this temperature range is consistent with a CuP_4 geometry. The sharp peak at *δ* 31 is most likely an impurity of the ligand bis-oxide. The minor peaks at *δ* 7, 22.5 and –6.8 are consistent with a neutral ring opened species [CuI(d2pype-*P*,*P*′)(d2pype-*P*)] (see text).

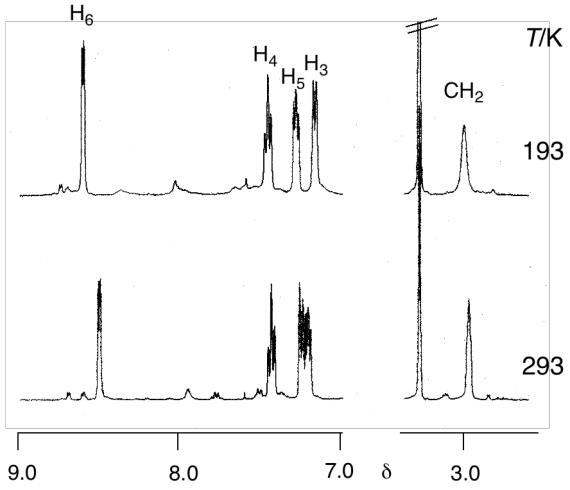

Fig. S5. 400 MHz ^{1}H NMR spectra of a 9.7 mM solution of [Cu(d2pype)$_2$]I in CD_3OD at 293 and 193 K (see also Fig. S6).

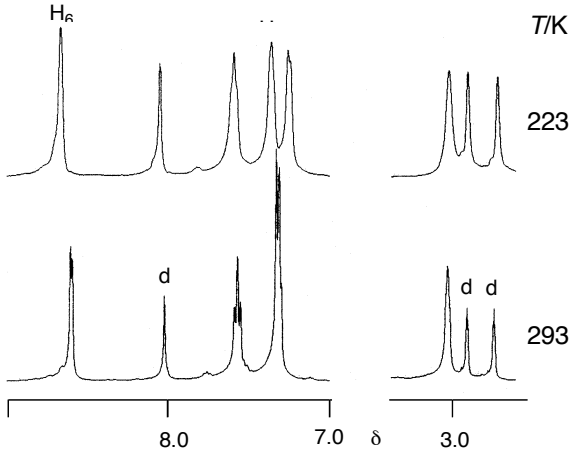

Fig. S6. 400 MHz ^{1}H NMR spectra of a 9.7 mM solution of [Cu(d2pype)$_2$]I in dmf-d_7 at 293 and 223 K. Resonances are assignable to the monomeric species and there is no evidence for the formation of high order assemblies such as dimer, trimer or tetramer. Peaks labeled "d" are the dmf solvent peaks