Electronic Supplementary Information

Supramolecular interaction of inositol phosphates with Cu(II): comparative study InsP_6-InsP_3

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Content

Table S1. Crystal data and refinement parameters for **1**·14 H_2O and **2**·10.5H_2O.

	1·14 H_2O	**2**·10.5H_2O
Empirical formula	$C_{66}H_{82}Cu_3N_{10}O_{39}P_6$	$C_{36}H_{56}Cu_2N_6O_{26.5}P_3$
Formula weight	2015.85	1216.85
Temperature (K)	298	100
space group	*$P2_1/c$*	*P-1*
a (Å)	10.5277(4)	14.6359(5)
b (Å)	30.222(1)	14.6677(5)
c (Å)	26.182(1)	15.1995(8)
α (°)	90	63.897(4)
β (°)	100.361(4)	64.765(4)
γ (°)	90	65.067(4)
Volume ($Å^3$)	8194.3(6)	2538.2(2)
Z	4	2
Independent reflections / R(int)	22869 / 0.0540	8712 / 0.0752
μ (mm^{-1})	0.990 (Mo-Kα)	2.754 (Cu-Kα)
R indices [I>2σ(I)]*	R1= 0.0844 wR2= 0.1999	R1= 0.0799 wR2= 0.2054
R indices (all data)*	R1= 0.1188 wR2= 0.2205	R1= 0.1113 wR2= 0.2659
CCDC no.	2129733	2129734

* $R1 = \Sigma \, || Fo| - |Fc|| / \Sigma \, |Fo|$; $wR2 = = [\Sigma w(Fo^2 - Fc^2)^2 / \Sigma \, wFo^4]^{½}$

Table S2. Bond distances (Å) and angles (deg) for metal coordination environments in **1**·14 H_2O.

Cu1 - N1	2.168(4)	Cu2 - N5	2.021(4)	Cu3 - N7	1.993(4)
Cu1 - N2	1.979(4)	Cu2 - N6	2.011(4)	Cu3 - N8	2.060(4)
Cu1 - N4	2.061(5)	Cu2 - O53	1.928(3)	Cu3 - N9	2.003(4)
Cu1 - N3	1.985(4)	Cu2 - O63	1.935(3)	Cu3 - N10	2.162(4)
Cu1 - O54	1.988(3)	Cu2 - OW1	2.328(4)	Cu3 - O43	1.958(3)
N1 - Cu1 - N2	80.5(2)	N5 - Cu2 - N6	81.4(2)	N7 - Cu3 - N8	81.9(2)
N1 - Cu1 - N4	118.0(2)	N5 - Cu2 - O53	167.8(2)	N7 - Cu3 - N9	174.0(2)
N1 - Cu1 - N3	94.0(2)	N5 - Cu2 - O63	90.9(2)	N7 - Cu3 - N10	99.2(2)
N1 - Cu1 - O54	101.8(2)	N5 - Cu2 - OW1	102.1(2)	N7 - Cu3 - O43	93.8(2)
N2 - Cu1 - N4	97.4(2)	N6 - Cu2 - O53	89.4(2)	N8 - Cu3 - N9	92.4(2)
N2 - Cu1 - N3	173.2(2)	N6 - Cu2 - O63	169.2(2)	N8 - Cu3 - N10	103.6(2)
N2 - Cu1 - O54	88.2(2)	N6 - Cu2 - OW1	93.1(2)	N8 - Cu3 - O43	155.1(2)
N4 - Cu1 - N3	81.7(2)	O53 - Cu2 - O63	97.1(2)	N9 - Cu3 - N10	80.2(2)
N4 - Cu1 - O54	140.2(2)	O53 - Cu2 - OW1	86.3(1)	N9 - Cu3 - O43	92.2(2)
N3 - Cu1 - O54	96.7(2)	O63 - Cu2 - OW1	95.9(1)	N10 - Cu3 - O43	101.3(2)

Table S3. Bond distances (Å) and angles (deg) for metal coordination environments in **2**·10.5H_2O.

Cu1 - N1	2.044(5)	Cu2 - N4	2.034(5)
Cu1 - N2	1.964(8)	Cu2 - N5	1.938(7)
Cu1 - N3	2.052(5)	Cu2 - N6	2.028(6)
Cu1 - O24	1.926(5)	Cu2 - OW1	1.944(7)
Cu1 - O34	2.184(5)	Cu2 - O14	2.145(5)
O24 - Cu1 - O34	98.8(2)	O14 - Cu2 - N4	99.4(2)
O24 - Cu1 - N1	95.5(2)	O14 - Cu2 - N5	92.7(2)
O24 - Cu1 - N2	162.0(2)	O14 - Cu2 - N6	92.6(2)
O24 - Cu1 - N3	103.4(2)	O14 - Cu2 - OW1	101.4(2)
O34 - Cu1 - N1	89.7(2)	N4 - Cu2 - N5	81.0(2)
O34 - Cu1 - N2	98.2(2)	N4 - Cu2 - N6	157.4(3)
O34 - Cu1 - N3	98.6(2)	N4 - Cu2 - OW1	99.3(2)
N1 - Cu1 - N2	79.1(3)	N5 - Cu2 - N6	79.3(3)
N1 - Cu1 - N3	157.8(2)	N5 - Cu2 - OW1	165.6(3)
N2 - Cu1 - N3	79.3(2)	N6 - Cu2 - OW1	97.0(3)

Table S4. PDB Identifiers and respective chemical names.

Identifier	*Name*
Monophosphates	
I4D	D-*myo*-Inositol-4-Phosphate
IPD	D-*myo*-Inositol-1-Phosphate
LIP	L-*myo*-Inositol-1-Phosphate
Bisphosphates	
2IP	D-*myo*-Inositol-1,4-Bisphosphate
IP2	D-*myo*-Inositol-4,5-Bisphosphate
ITP	Inositol 1,3-Bisphosphate
Trisphosphates	
FGV	D-*myo*-Inositol-1,3,5-Trisphosphate
I2P	D-*myo*-Inositol-2,4,5-Trisphosphate
I3P	D-*myo*-Inositol-1,4,5-Trisphosphate
I3S	(1S,3S,4S)-1,3,4-Triphospho-*Myo*-Inositol
Tetrakisphosphates	
4IP	Inositol-(1,3,4,5)-Tetrakisphosphate
4MY	*myo*-Inositol 3,4,5,6 Tetrakisphosphate
I0P	D-m*yo*-Inositol 1,4,5,6 Tetrakisphosphate
I4P	(1S,3R,4R,6S)-1,3,4,6-Tetrapkisphosphate
Pentakisphosphates	
5IP	D-*myo*-Inositol(1,2,3,5,6)-Pentakisphosphate
5MY	*myo*-Inositol-(1,3,4,5,6)-Pentakisphosphate
I5P	Inositol-(1,3,4,5,6)-Pentakisphosphate
IP5	D-*myo*-Inositol-(1,2,3,4,5)-Pentakisphosphate
K7V	*Neo*-Inositol Pentakisphosphate
Hexakisphosphates	
IHP	Inositol Hexakisphosphate
KGN	D-*Chiro* Inositol Hexakisphosphate

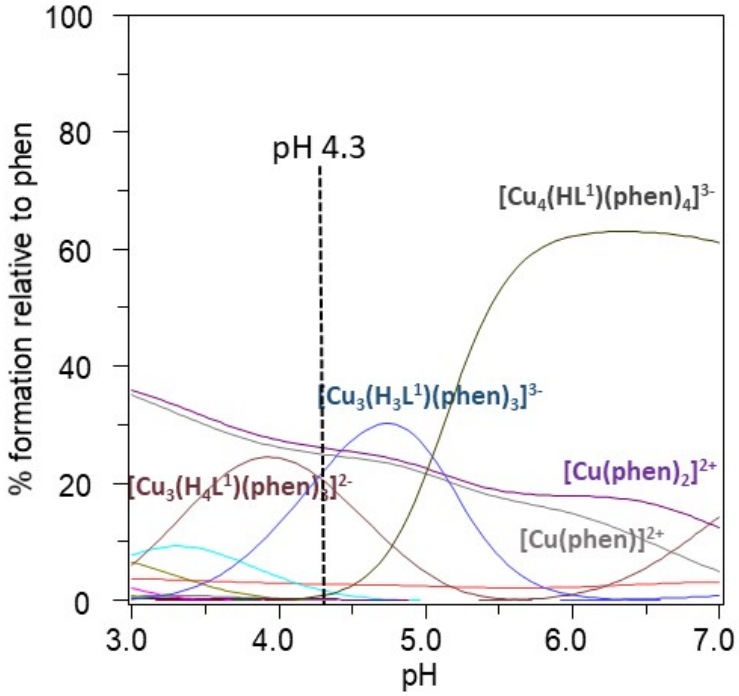

Fig. S1. Species distribution diagram for phen:L^1:Cu(II) system (in terms of phen percentage), in 0.15 M Me_4NCl at 37.0 °C from thermodynamic studies reported in [29]. Concentration of reactants follows those of the synthesis, [phen] = [Cu(II)] = 5 mM, [L^1] = 0.8 mM. The vertical dashed line represents the pH of synthesis.

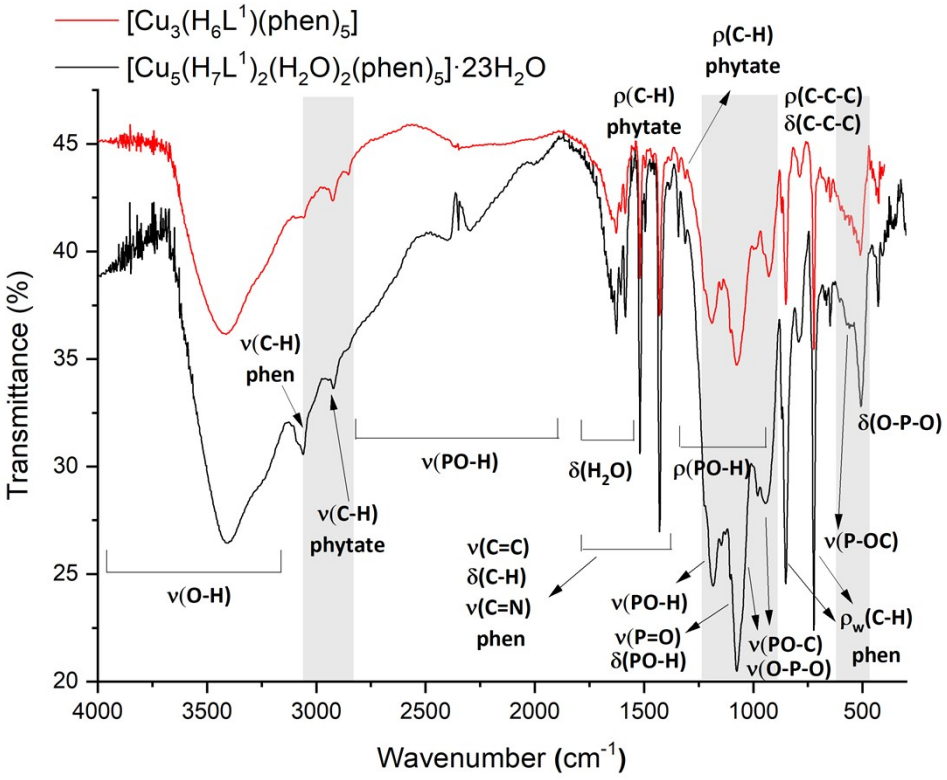

Fig. S2. Experimental IR spectra of complexes **1**·14H_2O and $[Cu_5(H_7L^1)_2(H_2O)_2(phen)_5]\cdot 23H_2O$ [29]. Grey zones highlight the slight differences between both spectra.

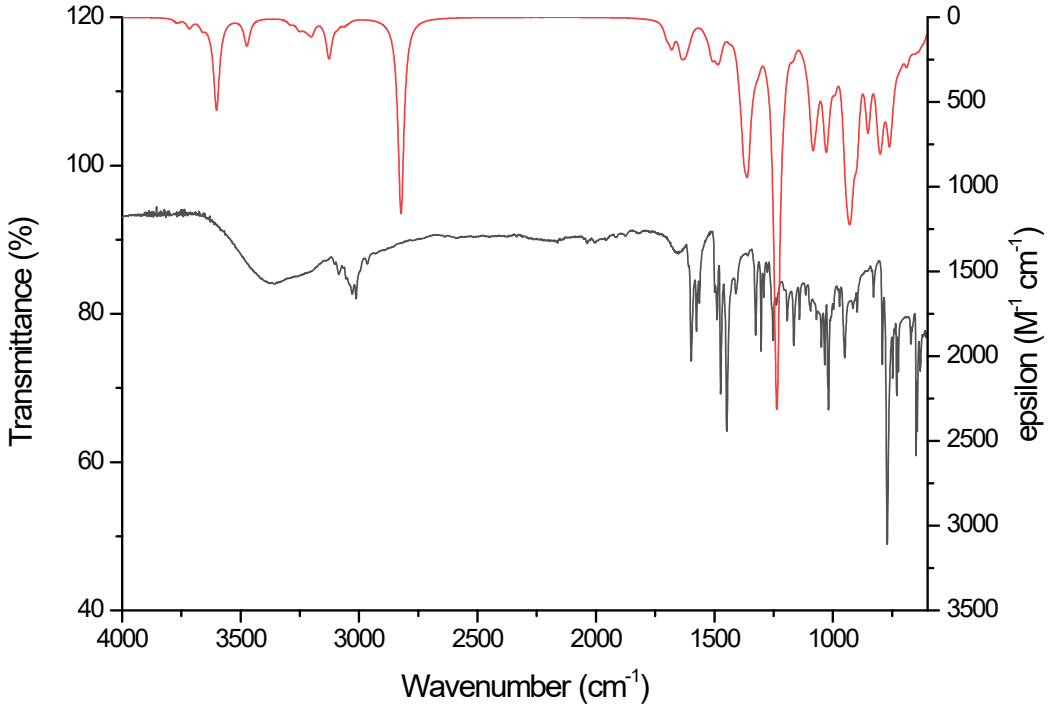

Fig. S3. Experimental (black) and theoretical (red) IR spectra of complex **2**.

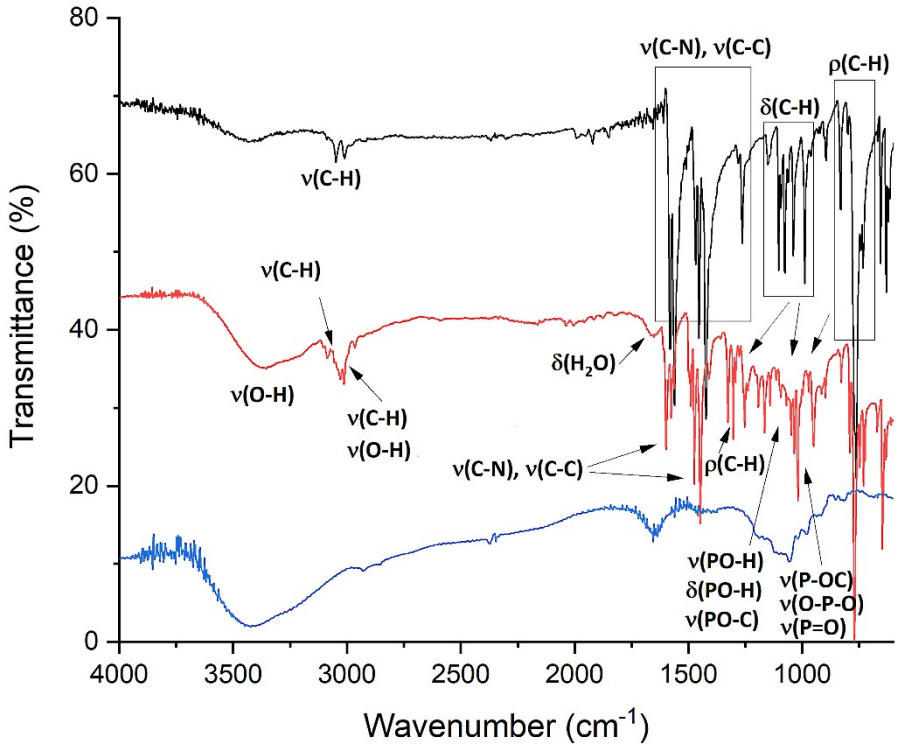

Fig. S4. Experimental IR spectra of compound **2**·10.5H_2O (red) and the ligands terpy (black) and sodium salt of L^2 (blue).

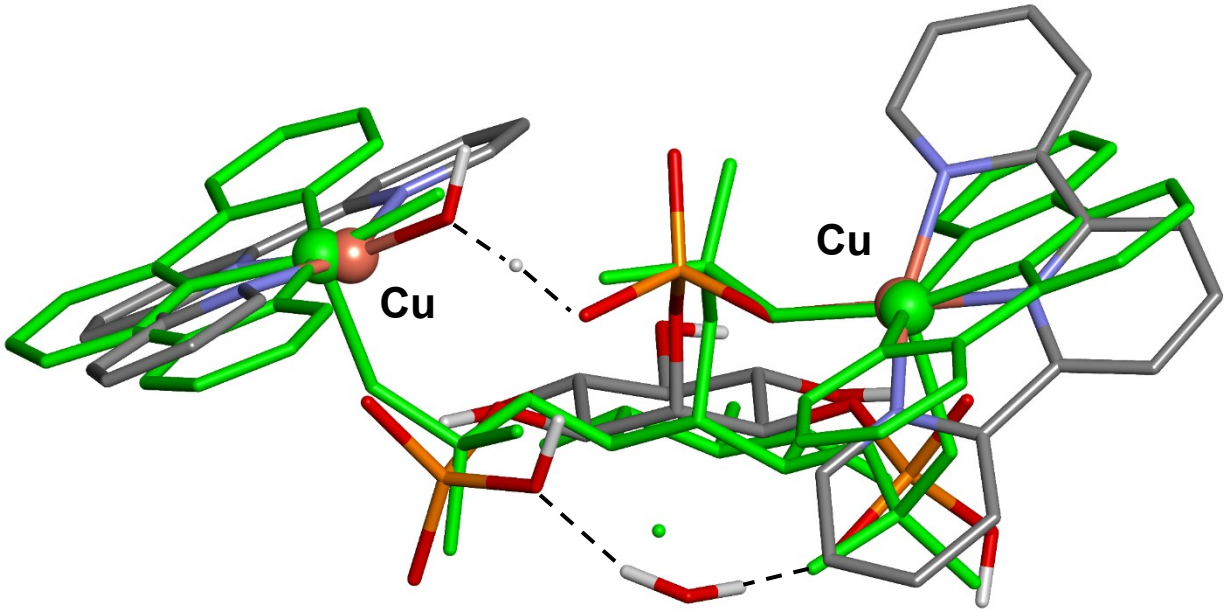

Fig. S5. DFT-optimized geometry in gas phase of **2**. Atom colour code: C (grey), O (red), N (blue), P (orange), Cu (pink). The corresponding crystal structure is shown superimposed in green. Non-polar hydrogen atoms are omitted for clarity.

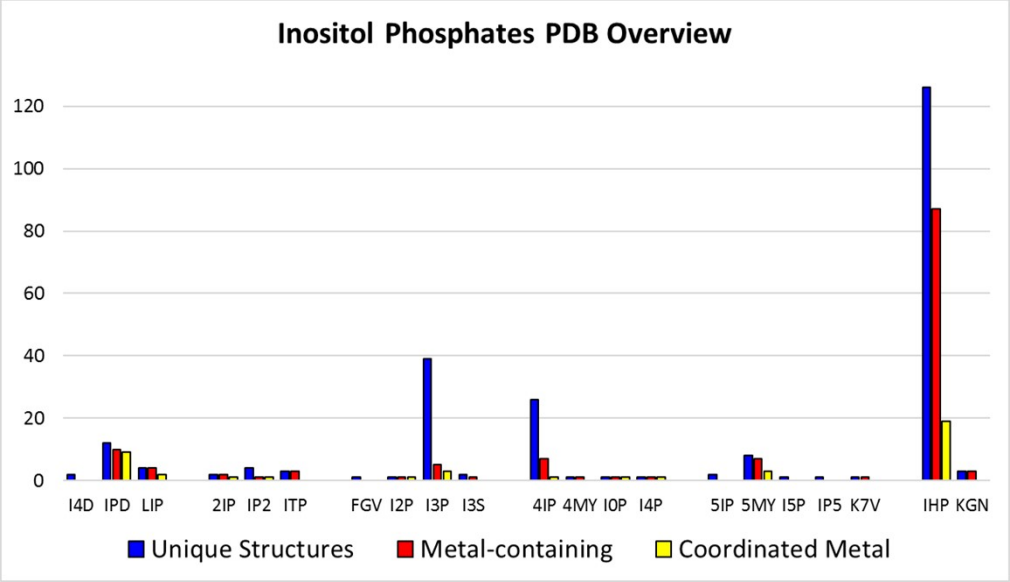

Fig. S6. Unique PDB structures containing inositol-phosphates (1-6 phosphate groups). Gaps separate isomers with different number of phosphate groups. Nomenclature follows PDB standard (cf. Table S4).

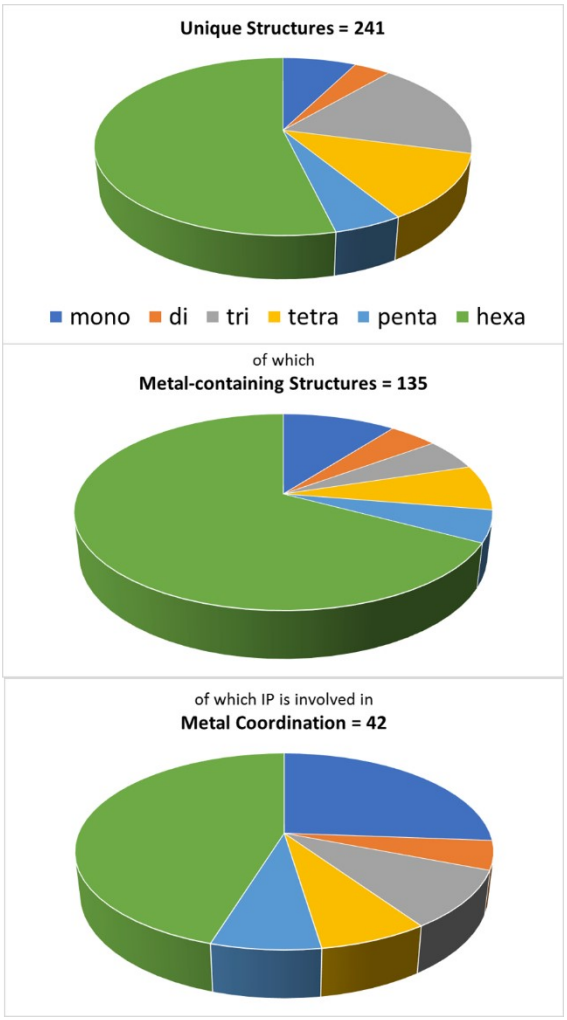

Fig. S7. Distribution of available literature material by number of phosphate substituents (1-6) on the inositol core.

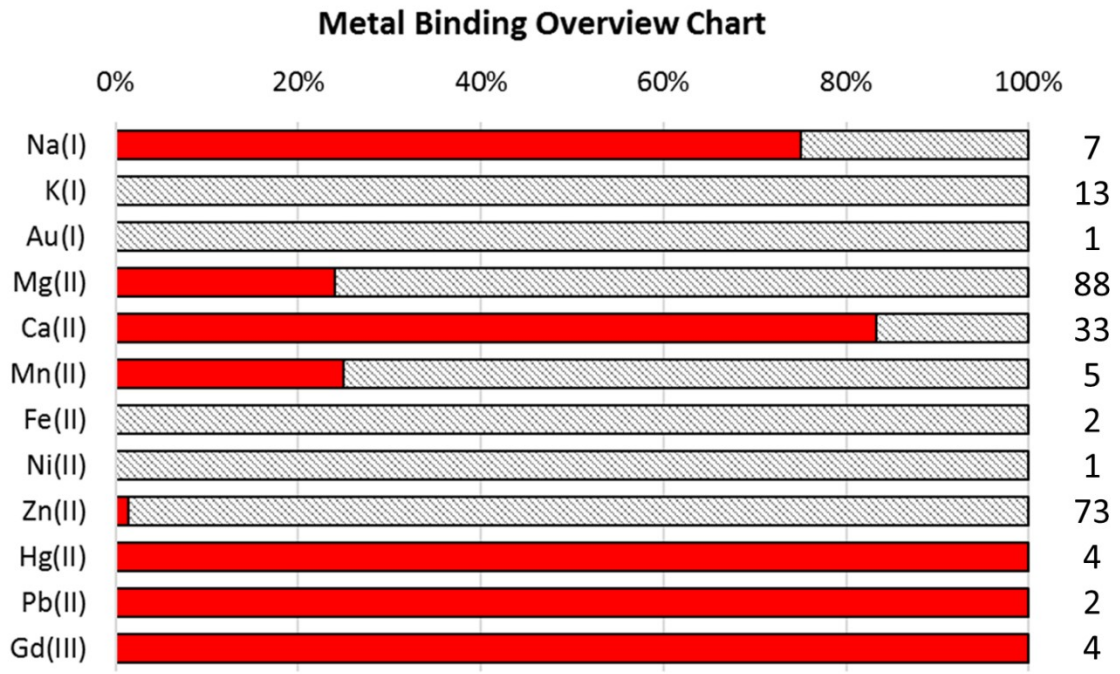

Fig. S8. Experimental metal by metal binding chance as percent of coordinated vs structure containing both the metal ion and Ins*P*s. Metal ions are sorted by charge, then by atomic number. Figures on the right are the number of PDB structures containing Ins*P*s and the specified metal cation.

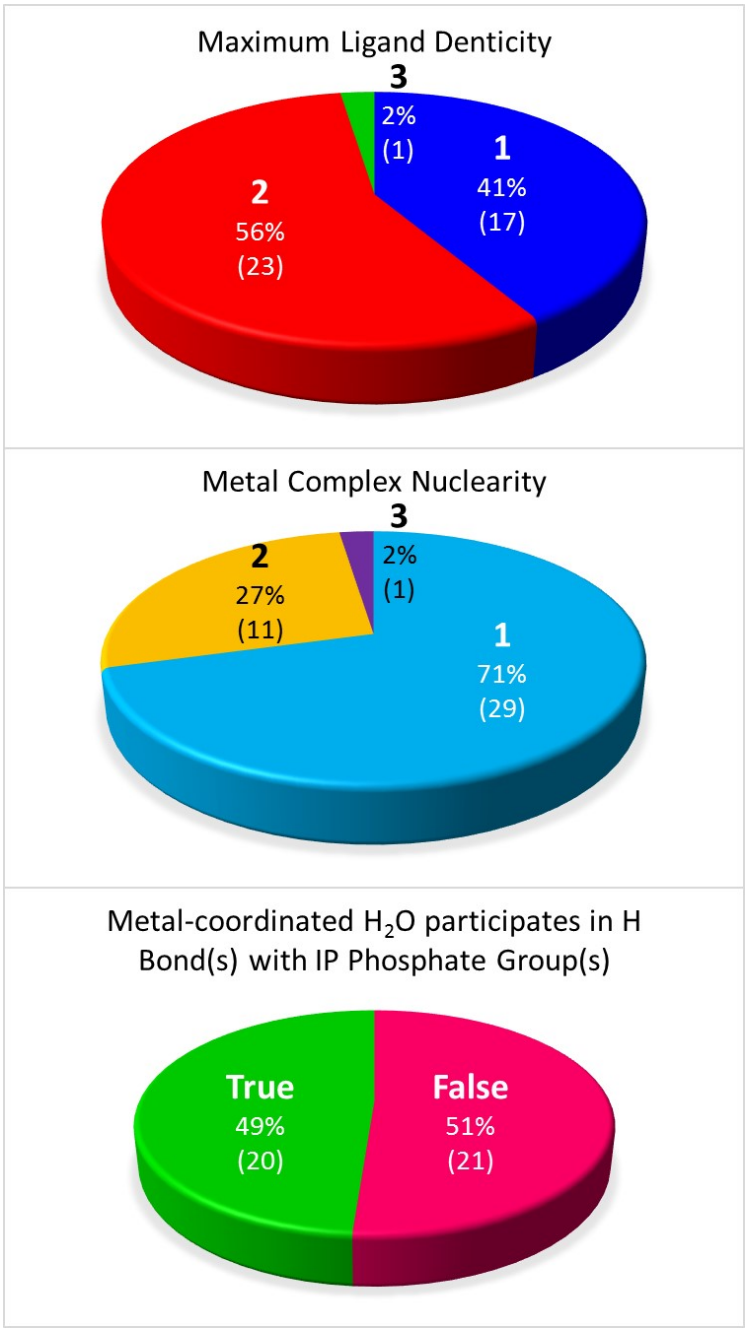

Fig. S9. Overlook on metal complexes features: ligand denticity, metal complex nuclearity (as number of metal cations directly bound to each Ins*P*), participations of metal-coordinated water molecules in H-bond with phosphate groups of the ligand.