Supplementary Material (ESI) for New Journal of Chemistry

Supplementary Material for:
Hydrophilic interior between hydrophobic regions in inverse bilayer structures of cation–1,1'-binaphthalene-2,2'-diyl phosphate salts

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This supplementary material contains the annotated pictures for the hydrogen-bonding interactions found in the crystal structures of the complexes (1,1'-binaphthalene-2,2'-diyl phosphate = BNPPA$^-$):

1 (Isonicotin-1-ium amide)-(*rac*-1,1'-binaphthalene-2,2'-diyl phosphate)·monohydrate, $(C_6H_7N_2O)(C_{20}H_{12}PO_4)\cdot H_2O$

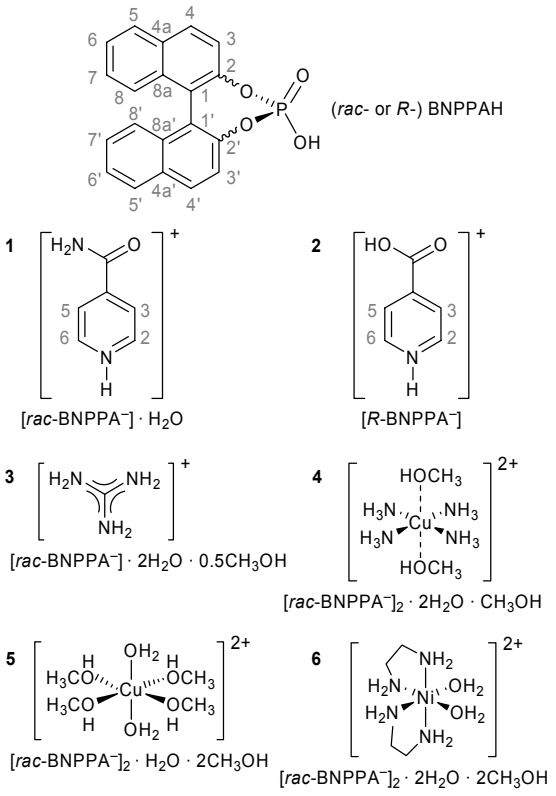
2 (Isonicotin-1-ium acid)-(*R*-1,1'-binaphthalene-2,2'-diyl phosphate), $(C_6H_6NO_2)(C_{20}H_{12}PO_4)$

3 (Guanidinium)-(*rac*-1,1'-binaphthalene-2,2'-diyl phosphate)·dihydrate·semimethanol, $(CH_6N_3)(C_{20}H_{12}PO_4)\cdot 2H_2O\cdot 0.5CH_3OH$

4 *trans*-[Tetraammin-di(methanol~0.75/aqua~0.25)-copper(II)]-bis(*rac*-1,1'-binaphthalene-2,2'-diylphosphate)·dihydrate·mono-methanol

5 *trans*-(Diaqua-tetramethanol-copper(II))-bis(*rac*-1,1'-binaphthalene-2,2'-diylphosphate)·hydrate·dimethanol

6 *cis*-[Diaqua-bis(ethylene diamine)-nickel(II)]-bis(*rac*-1,1'- binaphthalene-2,2'-diylphosphate)·dihydrate·dimethanol



Scheme 1 Molecular composition of the prepared 1,1'-binaphthalene-2,2'-diyl phosphate (BNPPA) salts **1-6** with the nomenclature numbering scheme.

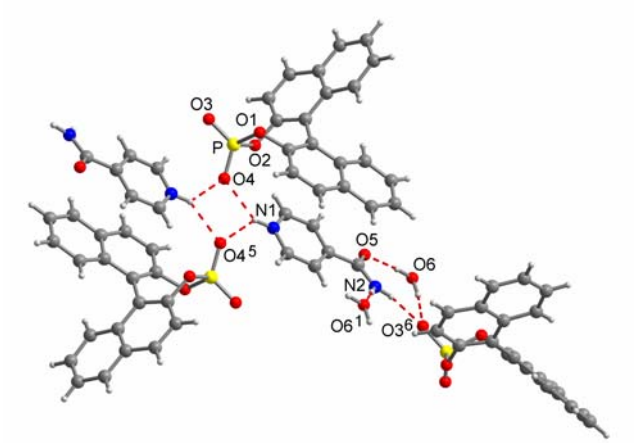


Fig. 1 Hydrogen bonding scheme in **1** (see Table 1 in paper for details).

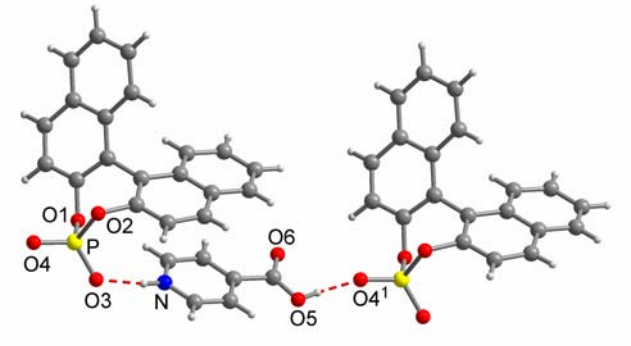


Fig. 2 Hydrogen bonding scheme in **2** (see Table 1 in paper for details).

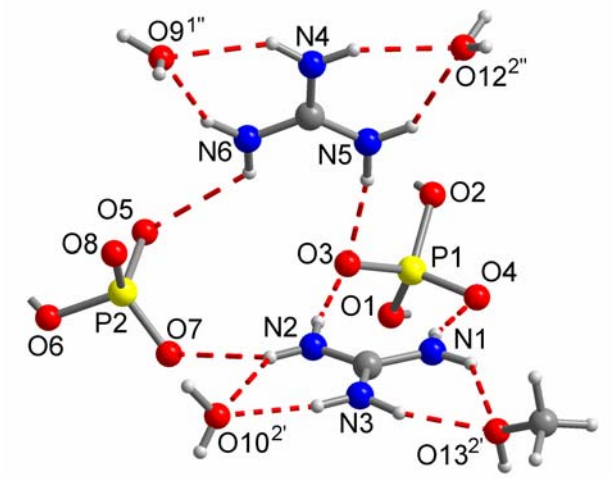


Fig. 3a Hydrogen bonding scheme around the guanidinium cation in **3** (see Table 2 in paper for details).

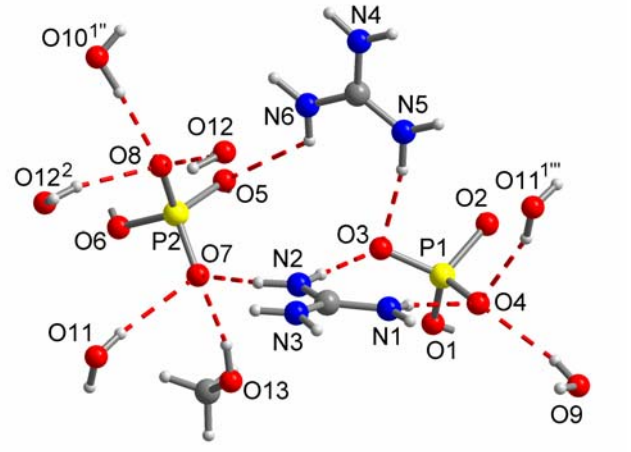


Fig. 3b Hydrogen bonding scheme around the phosphate head group of BNPPA in **3** (see Table 2 in paper for details). Additional symmetry transformation: 1''' = –1+x, y, z.

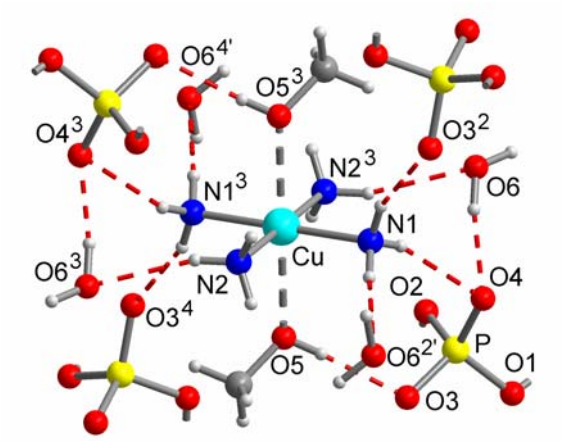


Fig. 4a Hydrogen bonding scheme around the complex *trans*-$[Cu(NH_3)_4(CH_3OH)_2]^{2+}$ in **4** (see Table 3 in paper for details). Additional symmetry transformation: 4 = x, 1/2–y, 1/2+z; 4' = x, 3/2–y, 1/2+z.

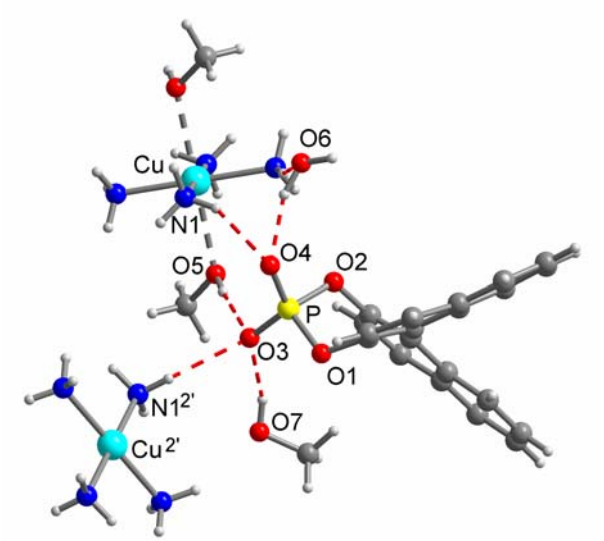


Fig. 4b Hydrogen bonding scheme around the phosphate head group of BNPPA in **4** (see Table 3 in paper for details). Additional symmetry transformation: 4 = x, 1/2–y, 1/2+z.

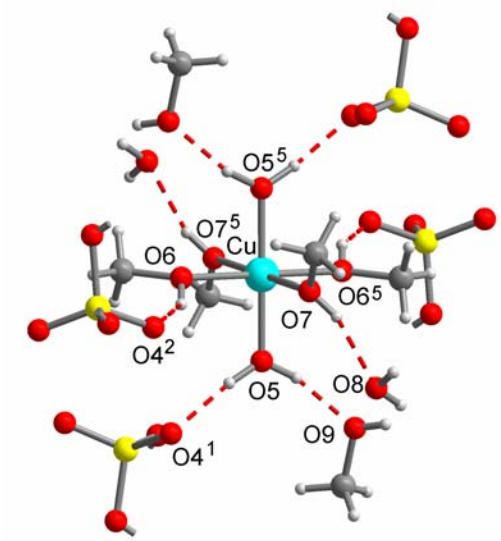


Fig. 5a Hydrogen bonding scheme around the complex *trans*-$[Cu(H_2O)_2(CH_3OH)_4]^{2+}$ in **5** (see Table 3 in paper for details). Additional symmetry transformation: 5 = –x, –y, –z

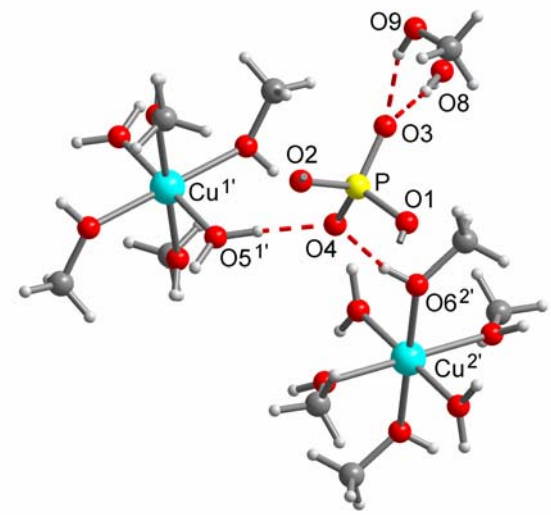


Fig. 5b Hydrogen bonding scheme around the phosphate head group of BNPPA in **5** (see Table 3 in paper for details). Additional symmetry transformations: 1' = x, 1+y, z; 2' = –x, 1+y, 1/2–z.

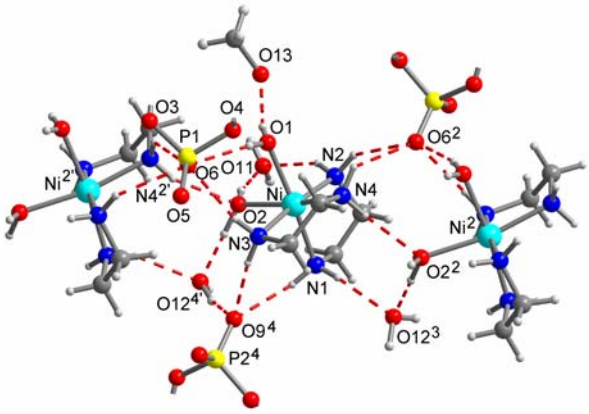


Fig. 6a Hydrogen bonding scheme around the complex *cis*-$[Ni(en)_2(H_2O)_2]^{2+}$ in **6** (see Table 4 in paper for details). Additional symmetry transformation: 2' = x, 1–y, 1/2+z.

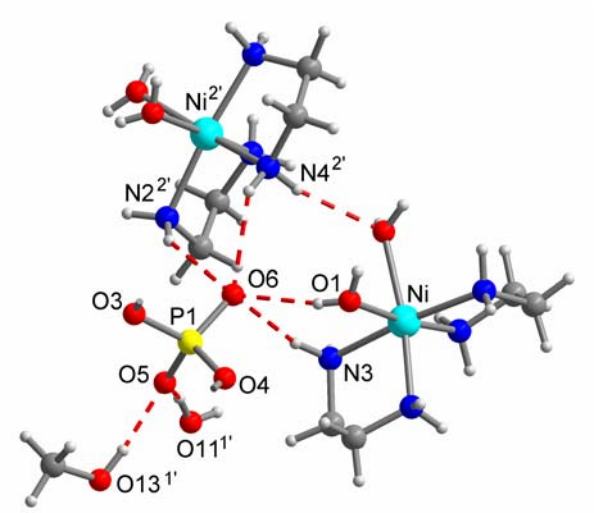


Fig. 6b Hydrogen bonding scheme around the phosphate head group with P1 of BNPPA in **6** (see Table 4 in paper for details). Additional symmetry transformations: 1' = x, –1+y, z; 2' = x, 1–y, 1/2+z.

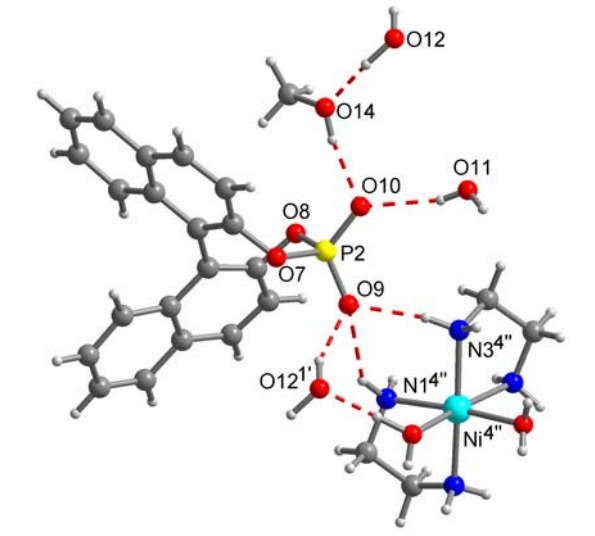


Fig. 6c Hydrogen bonding scheme around the phosphate head group with P2 of BNPPA in **6** (see Table 4 in paper for details). Additional symmetry transformations: 1' = x, –1+y, z; 4" = 1/2+ x, 1/2–y, 1/2+z.