Electronic Supplementary Information for Dalton Transactions


Supporting information

# A phosphorus-supported multisite coordination ligand containing three imidazolyl arms and its metalation behaviour. An unprecedented co-existence of mononuclear and macrocyclic dinuclear Zn(II) complexes in the same unit cell of a crystalline lattice.

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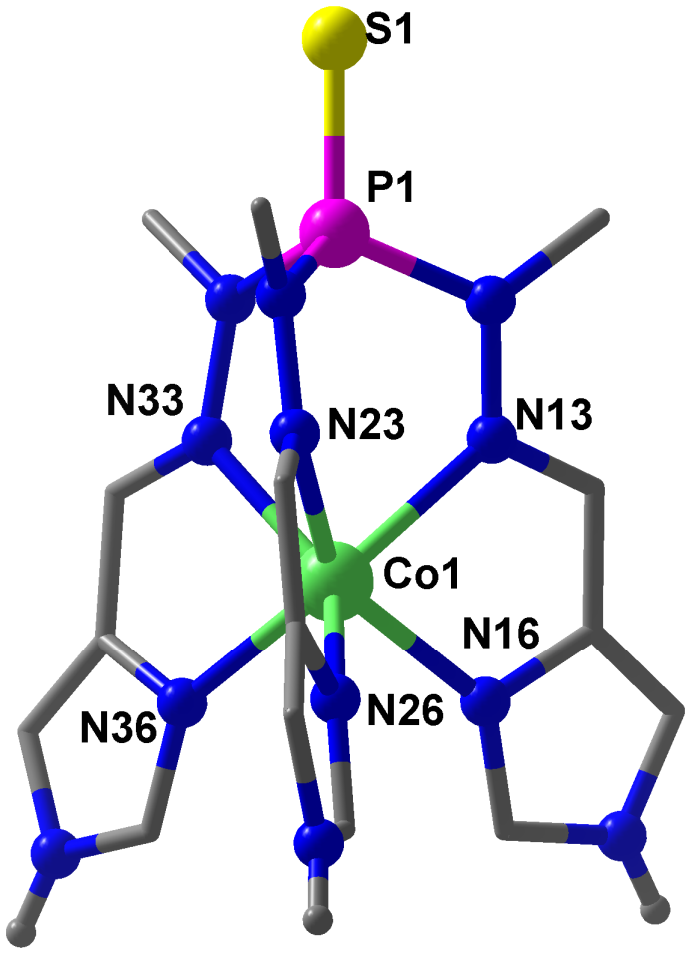


**Figure S1: Diamond view of cationic portion of 2.**

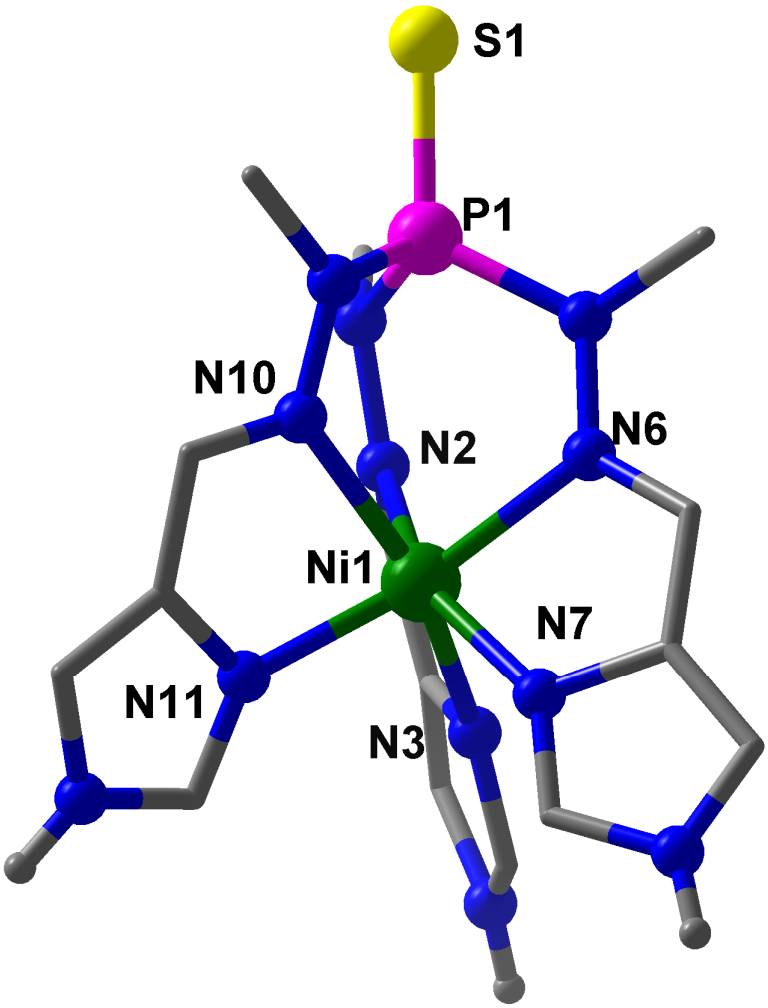


**Figure S2: Diamond view of cationic portion of 3.**

Table S1: Important hydrogen bonding bond parameters between imidazole hydrogen and nitrate oxygen.

| | H---O (Å) | N----O (Å) | N-H-O (º) | symmetry |
|---|---|---|---|---|
| H4N----O5 | 2.3703(57) | 2.9434(45) | 116.70(56) | -1+x, y, z |
| H20N---O4 | 2.0139(83) | 2.8438(83) | 167.55(71) | 1-x, 1-y, 1-z |
| H16N---O2 | 1.9166(68) | 2.7992(68) | 160.27(60) | X, y, z |
| H11N---O3 | 1.9541(58) | 2.8022(64) | 165.86 (47) | 1-x, y, z |

**Sheffield ChemPuter**

**Result of isotope pattern calculation**

Formula: $P_1S_1N_{12}H_{20}C_{15}Zn_1$

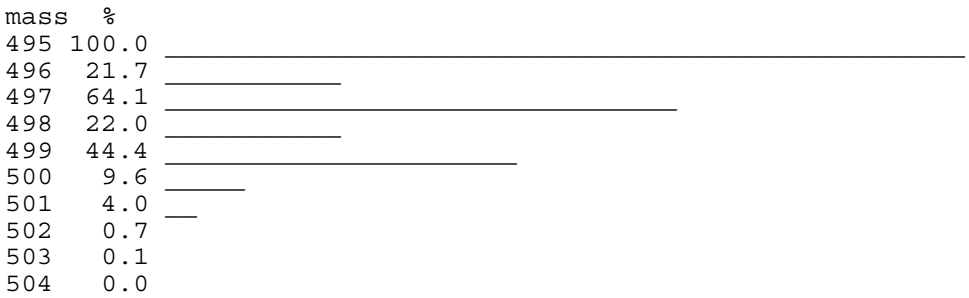


**Figure S3**: Sheffield chemputer generated isotopic pattern for [M-2$HNO_3$+$H^+$]

**Sheffield ChemPuter**

**Result of isotope pattern calculation**

Formula: $P_2S_2N_{24}H_{39}C_{30}Zn_2$

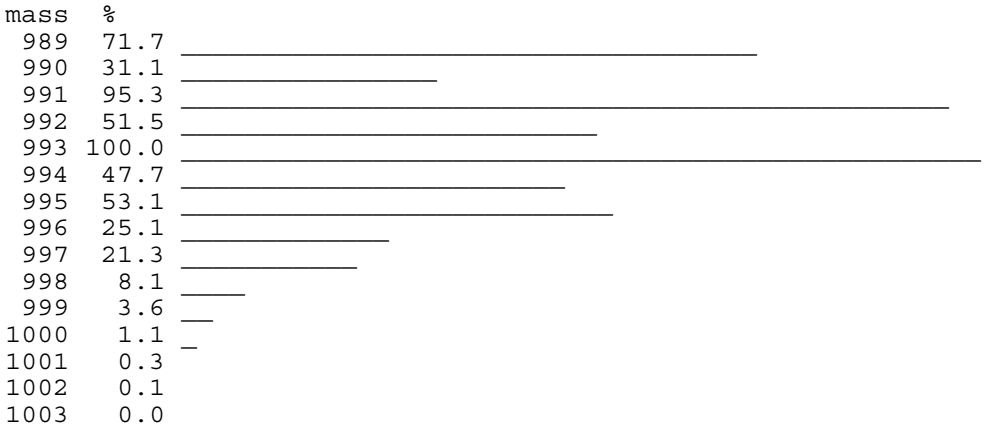


**Figure S4**: Sheffield chemputer generated isotopic pattern for [M-4$HNO_3$+$H^+$]