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RESEARCH COMMUNICATIONS

Novel coordination behaviour of *gem*-bis (pyrazolyl) cyclotriphosphazenes as tridentate NNN-donor ligands: The crystal structure of $[Mo(CO)_3\{N_3P_3Ph_4(3,5\text{-}Me_2C_3HN_2)_2\}]$

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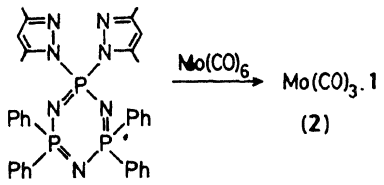
Reactions of group 6 metal carbonyls with bis(pyrazolyl) phosphazenes yield metal tricarbonyl complexes, $[M(CO)_3{\cdot}L]$ $[L = N_3P_3Ph_4(3,5\text{-}Me_2C_3HN_2)_2$ (1) or $N_3P_3(MeNCH_2CH_2O)_2(3,5\text{-}Me_2C_3HN_2)_2$ (4)]. The structure of the complex $[Mo(CO)_3{\cdot}1]$, determined by single-crystal X-ray analysis, shows that the (pyrazolyl) phosphazene acts as a tridentate ligand; the two pyridinic pyrazolyl nitrogen atoms and a phosphazene ring nitrogen atom are coordinated to the metal. A similar structure is proposed for the complexes $[M(CO)_3{\cdot}4]$ (M = Mo or W] on the basis of their spectroscopic data.

CURRENT interest in cyclophosphazenes is mainly focused on their organometallic chemistry[1,2]. Zerovalent metal complexes of cyclotriphosphazenes are sparse and have not been structurally characterized[1,3]. In this communication, we report the synthesis and structural study of the molybdenum tricarbonyl complex **2** of 2,2,4,4-tetraphenyl-6, 6-bis(3,5-dimethyl-1-pyrazolyl) cyclotriphosphazene (**1**) in which a phosphazene ring nitrogen atom is involved in coordination along with the two pyrazolyl pyridinic nitrogen atoms. We also report the synthesis and spectroscopic studies of a new bis(pyrazolyl) cyclotriphosphazene, viz. 2,2,4,4-bis (*N*-methylethanolamino)-6,6-bis(3,5-dimethyl-1-pyrazolyl) cyclotriphosphazene (**4**) and its metal tricarbonyl complexes, $[M(CO)_3{\cdot}4]$ (M = Mo (**5a**) or W (**5b**)). Complexes **2** and **5** are the first examples of structurally well-characterized systems in which a cyclotriphosphazene acts as a tridentate ligand. Pd(II) and Pt(II) complexes of pyrazolylphosphazenes are known but in these complexes there is no involvement of phosphazene ring nitrogen atom in coordination[4].



Compound **2** was prepared by heating[4] the ligand **1** (0.5 g) and molybdenum hexacarbonyl (0.2 g) (molar ratio 1:1) in 40 ml acetonitrile under reflux in an atmosphere of dry N_2 for 6 h. The product was precipitated as yellow crystals, which was washed with acetonitrile and dried under vacuum (yield: 76%). Single crystals were obtained by carrying out the reaction under appropriate dilute conditions and cooling the reaction mixture to 0°C. Compound **2** is not soluble in common organic solvents. Elemental analyses and infrared spectrum showed it to be a metal tricarbonyl derivative, $[Mo(CO)_3 \cdot 1]$. The structure of the complex was determined by single-crystal X-ray diffraction and a view of the molecule is shown in Figure 1. In addition to the pyridyl nitrogen atoms of the pyrazolyl groups, a nitrogen atom of the phosphazene ring is involved in coordination to the metal.

The geometry around the metal atom is distorted octahedral with short M–C bonds on one face and longer M–N bonds on the opposite face. The metallocycle is in a boat form and the heads of the boat (P1 and Mo) are bridged by a phosphazene ring nitrogen atom. The phosphazene ring is distinctly non-planar; the phosphorus atom (P3) and the adjascent nitrogen atom (N2) project upward (by 0.17 Å) from the plane formed by the other phosphazene ring atoms (N3, P1, N1, P2). The phosphorus-nitrogen bond distances are in the range 1.557(2)–1.637(2) Å with a mean value 1.600 Å. The phosphazene ring nitrogen–metal bond is longer (2.394(2) Å) than the pyrazolyl nitrogen–metal