Electronic supplementary materials *Mendeleev Commun.*, 2012, **22**, 187–188

Tris(2-pyridyl)phosphine: a straightforward microwave-assisted synthesis from 2-bromopyride and red phosphorus and coordination with cobalt(II) dichloride

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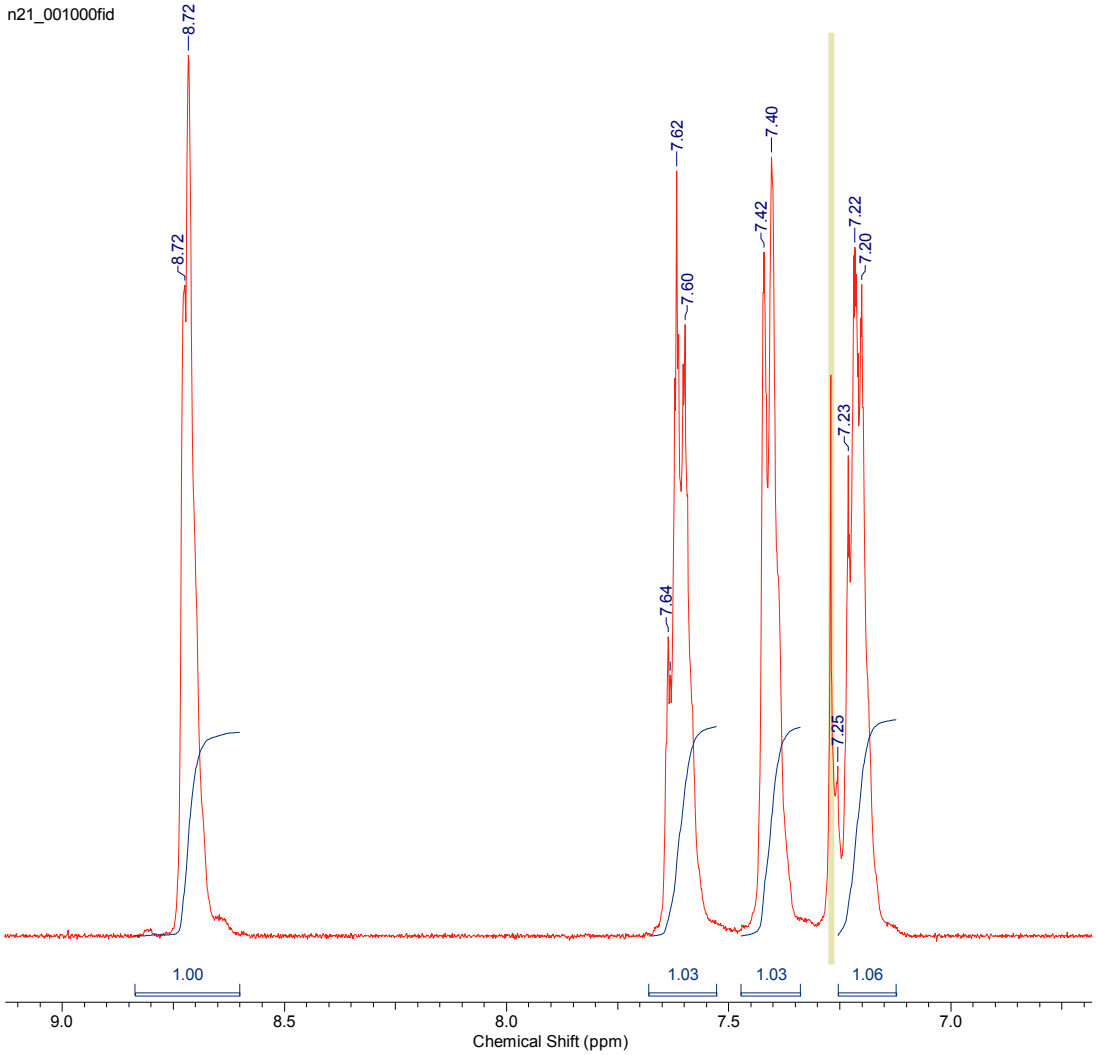
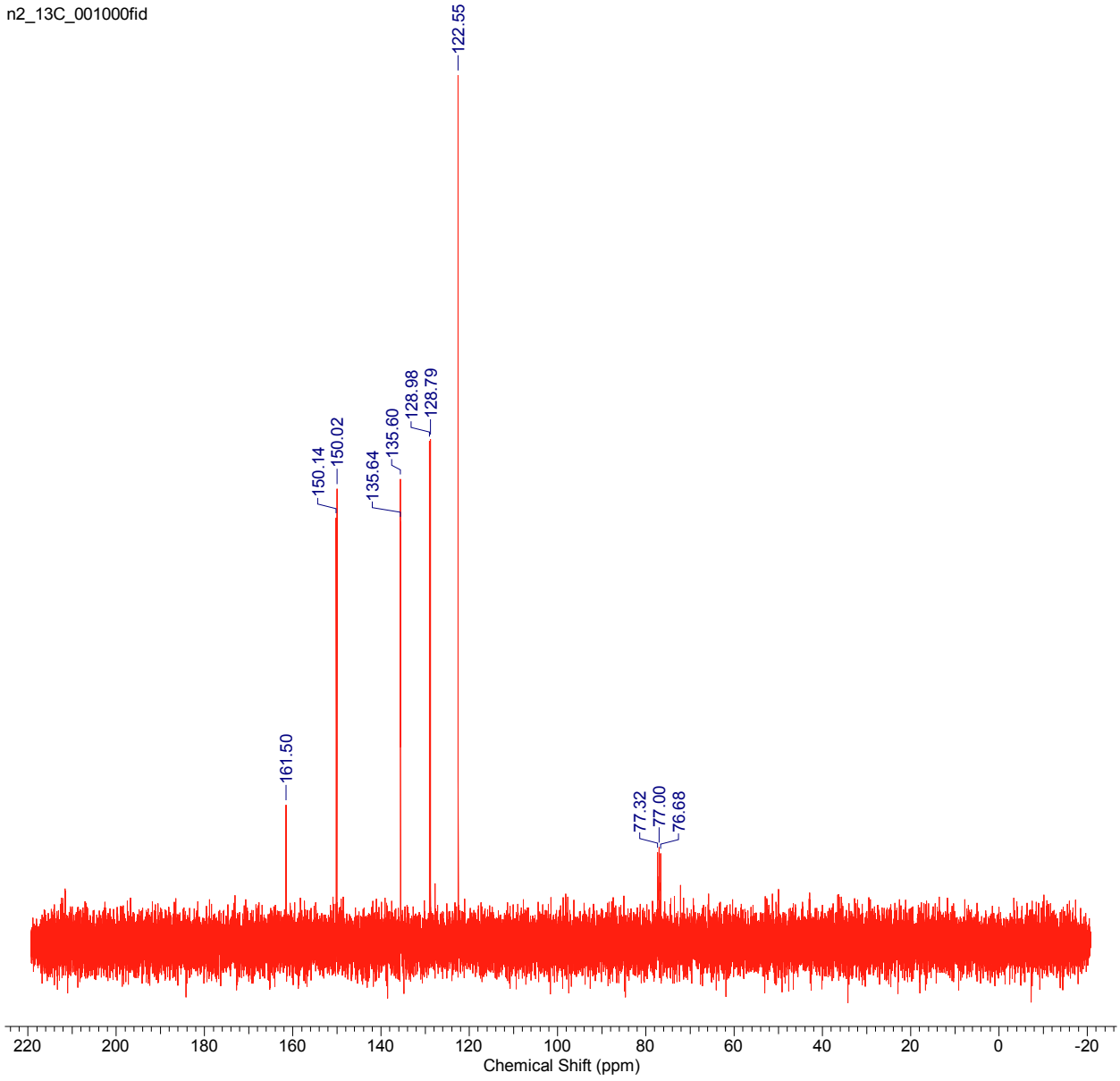
^{1}H, ^{13}C and ^{31}P NMR spectra of tris(2-pyridyl)phosphine

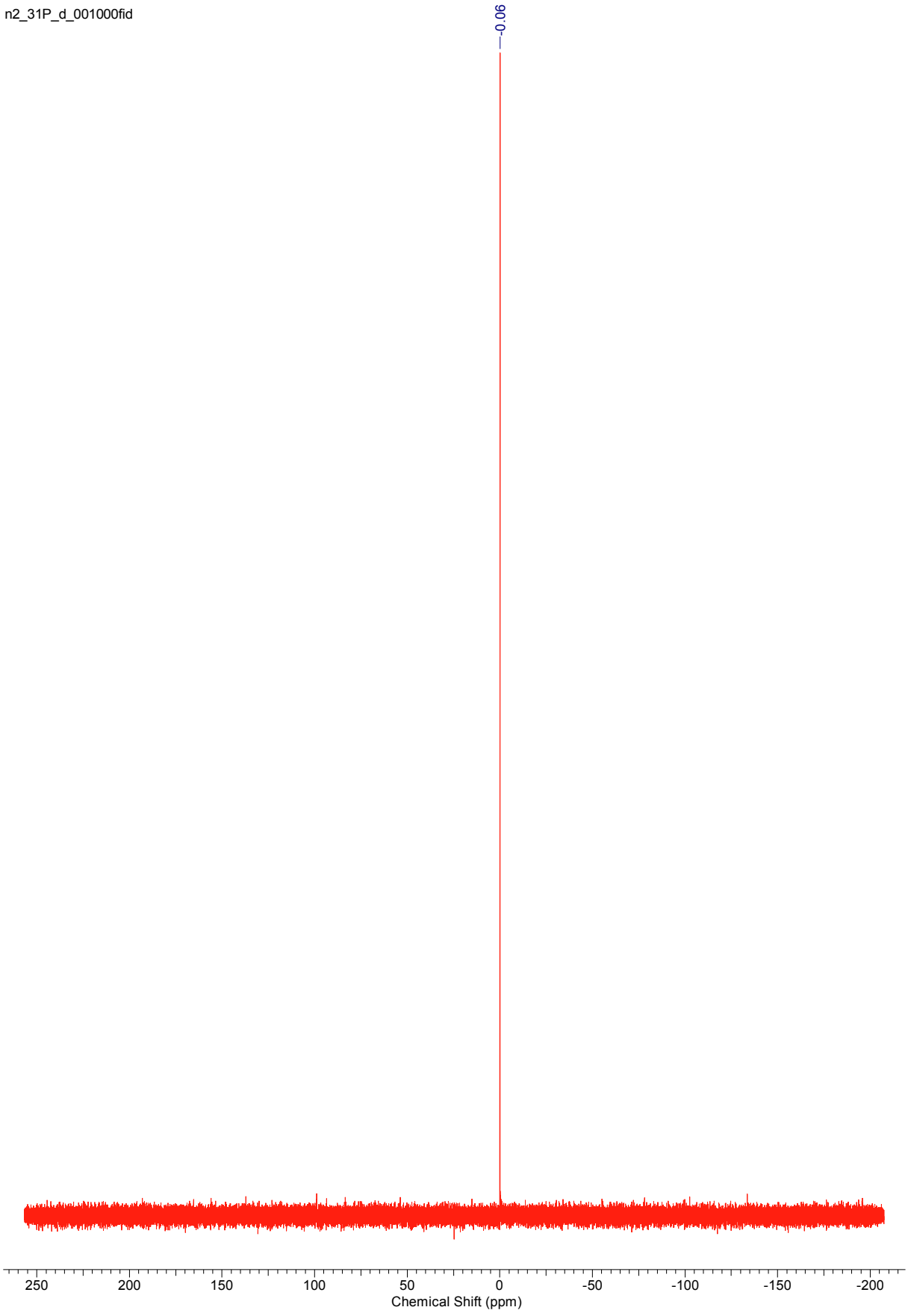
^{1}H NMR spectrum of tris(2-pyridyl)phosphine (in $CDCl_3$ solution)



^{13}C NMR spectrum of tris(2-pyridyl)phosphine (in $CDCl_3$ solution)



^{31}P NMR spectrum of tris(2-pyridyl)phosphine (in $CDCl_3$ solution)



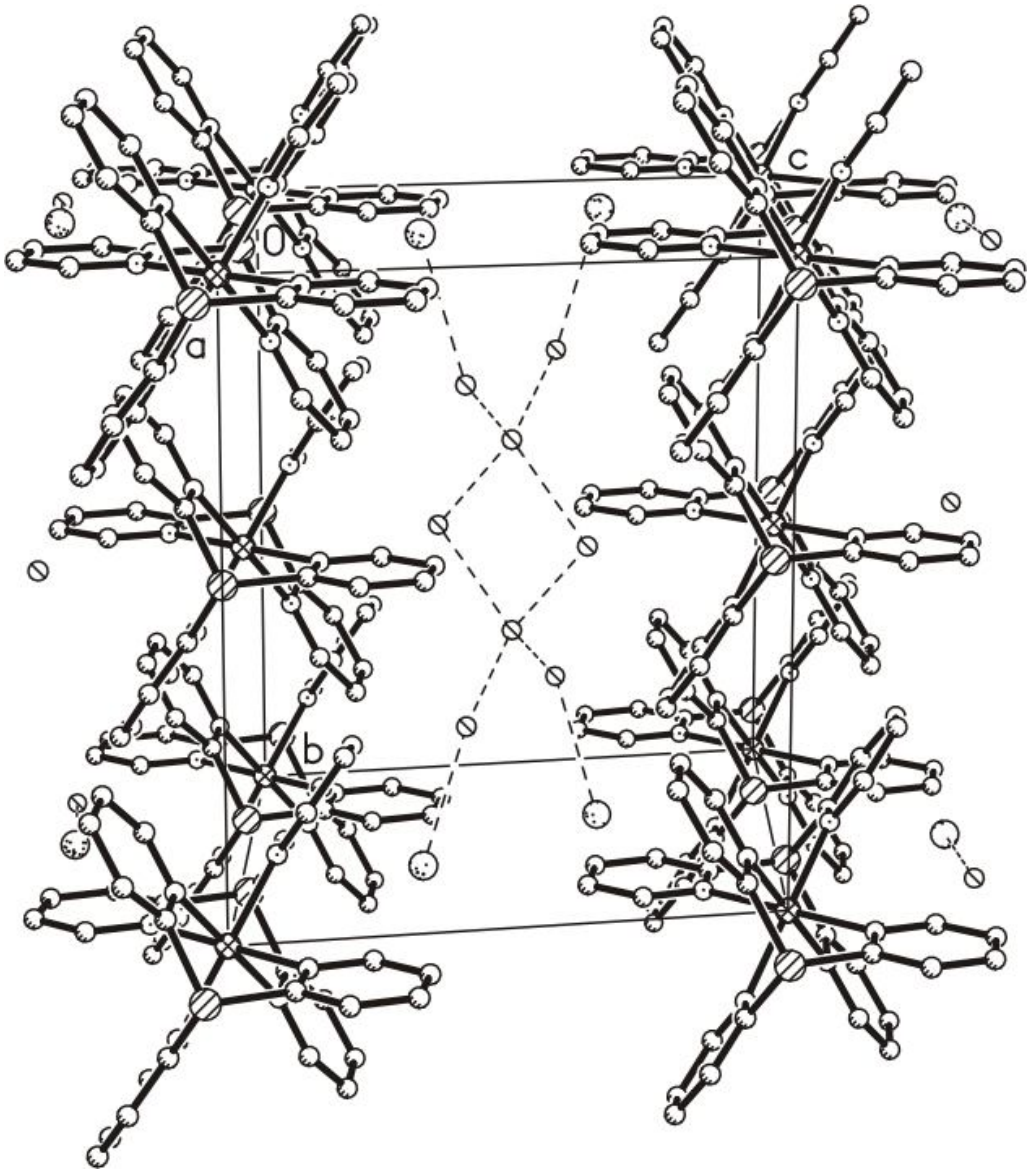


Figure 1S The crystalline structure of complex $[Co(2\text{-}Py_3P)_2]Cl_2 \cdot 8H_2O$ (**2**). It should be noted that short intermolecular contacts exist between chloride anions and water molecules as is evident from the Cl…O distances of 3.171(1) and 3.236(1) Å, which is less than the sum of the van der Waals radii (3.27 Å).[1]

References

1. A. Bondi, *J. Phys. Chem.*, 1964, **68**, no 3, 441.

Table 1S Bond distances (Å) for complex **2**.

Co(1)-P(1)	3.4840(5)
Co(1)-N(2)	2.1449(12)
Co(1)-N(1)	2.1614(9)
P(1)-C(10)	1.8387(15)
P(1)-C(5)	1.8405(11)
N(1)-C(1)	1.3442(14)
N(1)-C(5)	1.3508(13)
N(2)-C(6)	1.343(2)
N(2)-C(10)	1.3537(18)
C(1)-C(2)	1.3845(17)
C(2)-C(3)	1.3834(18)
C(3)-C(4)	1.3920(17)
C(4)-C(5)	1.3859(15)
C(6)-C(7)	1.393(2)
C(7)-C(8)	1.383(2)
C(8)-C(9)	1.387(2)
C(9)-C(10)	1.392(2)

Table 2S Bond angles (°) for complex **2**.

N(2)-Co(1)-N(2)#1	180.0
N(2)-Co(1)-N(1)#1	92.24(3)
N(1)#1-Co(1)-N(1)#2	88.62(5)
N(2)-Co(1)-N(1)	87.77(3)
N(2)#1-Co(1)-N(1)	92.23(3)
N(1)#1-Co(1)-N(1)	180.0
N(1)#2-Co(1)-N(1)	91.38(5)
N(1)#1-Co(1)-N(1)#3	91.39(5)
C(10)-P(1)-C(5)	101.14(4)
C(5)-P(1)-C(5)#3	98.68(6)
C(1)-N(1)-C(5)	117.59(9)
C(1)-N(1)-Co(1)	119.55(7)
C(5)-N(1)-Co(1)	122.59(7)
C(6)-N(2)-C(10)	118.07(13)
C(6)-N(2)-Co(1)	119.94(10)
C(10)-N(2)-Co(1)	121.99(10)
N(1)-C(1)-C(2)	123.48(10)
C(3)-C(2)-C(1)	118.67(11)
C(2)-C(3)-C(4)	118.56(11)
C(5)-C(4)-C(3)	119.41(10)
N(1)-C(5)-C(4)	122.25(10)
N(1)-C(5)-P(1)	121.33(8)
C(4)-C(5)-P(1)	116.37(8)
N(2)-C(6)-C(7)	122.85(14)
C(8)-C(7)-C(6)	119.01(15)
C(7)-C(8)-C(9)	118.55(14)
C(8)-C(9)-C(10)	119.61(14)
N(2)-C(10)-C(9)	121.91(14)
N(2)-C(10)-P(1)	122.36(11)
C(9)-C(10)-P(1)	115.73(11)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z #2 -x,y,-z #3 x,-y,z