Synthesis and structure of small-molecule phosphazene rings bearing fused-ring aryloxy side groups: models for optically useful high polymers (1995, 3521)

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The crystal structure of compound **6b** reported in the paper has been assigned the space group *P*1 in error. The correct space group is tetragonal *I*4 which can be transformed from the triclinic space group by the matrix:

$$\begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}$$

Crystal data: $C_{80}H_{56}N_4O_8P_4 \cdot C_6H_{14}$, $M = 1411.42$, tetragonal, space group $I\bar{4}$, $a = 15.652(9)$, $c = 14.197(5)$ Å, $U = 3478(2)$ Å^3, $Z = 2$, $D_c = 1.35$ Mg m^{-3}, λ(Mo-Kα) = 0.710 69 Å, $\mu = 1.73$ mm^{-1}, $R = R' = 0.0446$ for 1507 observed data with $I > 3\sigma(I)$ and 223 parameters.

After performing the transformation and merging the data, the structure (see Fig. 1) was refined by full-matrix least-squares calculations with anisotropic displacement parameters for non-hydrogen atoms except solvent C-atoms which were disordered and allowed isotropic thermal parameters. Hydrogen atoms of the naphthyloxy group were included at geometrically idealized positions with C–H 0.95 Å; solvent H-atoms were ignored. In the last refinement cycle, shifts were 0.00 and the final difference map was featureless. The revised positional parameters and molecular dimensions are given in Tables 1 and 2, respectively.

Atomic coordinates, thermal parameters, and bond lengths and angles have been deposited at the Cambridge Crystallographic Data Centre (CCDC). See Instructions for Authors, *J. Chem. Soc., Dalton Trans.*, 1996, Issue 1. Any request to the CCDC for this material should quote the full literature citation and the reference number 186/114.

The authors sincerely thank Professor Ivan Bernal for suggesting the transformation of triclinic to tetragonal space group.

Table 1 Positional parameters for compound **6b**

Atom	*x*	*y*	*z*
P(1)	0.373 28(6)	0.040 44(6)	0.251 6(1)
O(1)	0.317 2(2)	0.072 1(2)	0.164 8(3)
O(2)	0.312 2(2)	0.044 0(2)	0.339 9(3)
N(1)	0.391 6(2)	−0.056 0(2)	0.235 8(3)
C(1)	0.258 1(3)	0.017 4(3)	0.119 8(4)
C(2)	0.182 8(4)	−0.000 8(4)	0.163 0(5)
C(3)	0.123 3(4)	−0.052 6(5)	0.113 8(8)
C(4)	0.142 4(7)	−0.080 6(5)	0.025 9(9)
C(5)	0.219 4(6)	−0.062 9(4)	−0.017 9(6)
C(6)	0.242 7(8)	−0.090 6(6)	−0.112 5(7)
C(7)	0.315 5(10)	−0.068 3(9)	−0.152 1(8)
C(8)	0.373 7(7)	−0.019 8(6)	−0.104 4(7)
C(9)	0.359 1(5)	0.008 9(5)	−0.014 6(5)
C(10)	0.281 3(4)	−0.011 0(3)	0.029 7(5)
C(11)	0.278 4(3)	0.119 4(3)	0.382 6(4)
C(12)	0.268 0(3)	0.192 7(4)	0.337 5(5)
C(13)	0.232 5(4)	0.262 8(4)	0.386 5(6)
C(14)	0.206 5(4)	0.251 6(5)	0.476 7(6)
C(15)	0.216 0(4)	0.176 0(5)	0.524 2(5)
C(16)	0.187 9(6)	0.165 5(7)	0.621 0(7)
C(17)	0.199 1(7)	0.086 8(8)	0.662 5(7)
C(18)	0.237 1(6)	0.020 6(8)	0.616 7(5)
C(19)	0.264 7(5)	0.026 4(4)	0.525 0(5)
C(20)	0.253 3(3)	0.106 7(4)	0.476 6(4)
C(21)	1.000 0	0.000 0	0.349 3(12)
C(22)	1.030 3(10)	0.017 8(12)	0.447 7(8)

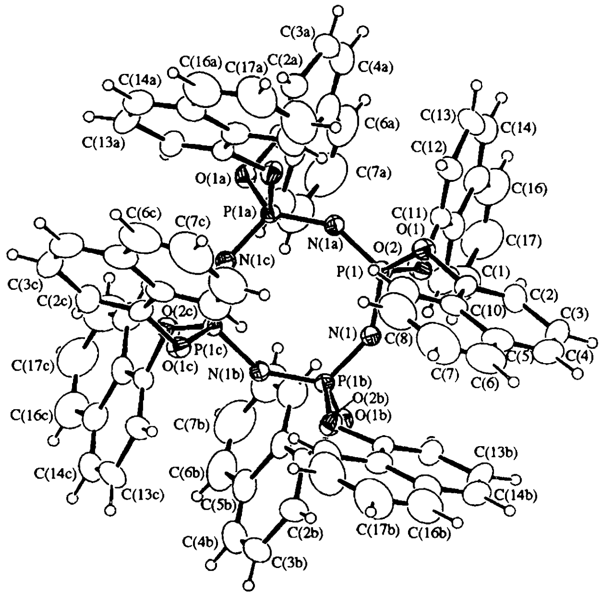

Fig. 1 Revised Fig. 11 (molecular structure of **6b**). The symmetry codes are: a $y + 0.5$, $-x + 0.5$, $-z + 0.5$; b $-y + 0.5$, $x - 0.5$, $-z + 0.5$ and c $-x + 1$, $-y$, z

Table 2 Selected bond lengths (Å) and angles (°) for compound **6b***

P(1)–O(1)	1.592(4)	P(1)–O(2)	1.577(4)	O(1)–C(1)	1.413(6)
P(1)–N(1)	1.553(3)	P(1)–N(1a)	1.545(3)	O(2)–C(11)	1.428(6)
O(1)–P(1)–O(2)	105.6(2)	O(1)–P(1)–N(1)	107.1(2)	P(1)–N(1a)–P(1a)	143.7(2)
O(1)–P(1)–N(1a)	105.7(2)	O(2)–P(1)–N(1)	105.1(2)	O(1)–C(1)–C(10)	115.8(5)
O(2)–P(1)–N(1a)	108.5(2)	N(1)–P(1)–N(1a)	123.6(2)	O(1)–C(1)–C(2)	119.4(6)
P(1)–O(1)–C(1)	121.5(3)	P(1)–O(2)–C(11)	126.3(3)	O(2)–C(11)–C(20)	112.9(5)

* Atoms a related to the reference atoms by symmetry: $y + 0.5$, $-x + 0.5$, $-z + 0.5$.

Diiron(III) and polymeric iron(III)–sodium complexes with bridging and terminal pyridonate ligands: structures and magnetic properties (1996, 321)

Alexander J. Blake, Craig M. Grant, Simon Parsons, Gregory A. Solan and Richard E. P. Winpenny

The magnetic data reported for compounds **2** and **3** are misinterpreted due to a mistake in the computer modelling of the experimental data. The correct J values are -12.9 and -13.8 cm^{-1} for **2** and **3** respectively.
Page 327. Ref. 12 should read: F. E. Mabbs and D. J. Machin, *Magnetism and Transition Metal Complexes*, Chapman and Hall, London, 1973.