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*P*1 or $P\bar{1}$? Corrigendum

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The structure of bis((phenyl-*O*,*N*,*N*-azoxy)oxy)-methane, $C_{13}H_{12}N_4O_4$, originally reported as triclinic, space group *P*1 [Zyuzin *et al.* (1997). *Isz. Akad. Nauk SSSR Ser. Khim.* pp. 1486–1492; CSD refcode NIXQAM] was recently revised to monoclinic, space group *C*2 [Marsh (1999). *Acta Cryst.* B**55**, 931–936]. It is properly described as orthorhombic, space group *Fdd*2.

1. Comment

In a recent survey (Marsh, 1999) of structures reported in the Cambridge Structural Database (1992) as belonging to space group *P*1, but which should be described in higher symmetries, I noted that the entry under Refcode NIXQAM should be revised from *P*1 ($Z = 2$) to *C*2 ($Z = 4$). Dr Anthony Spek has now advised me that even higher symmetry is present in the structure and that it is properly described as orthorhombic, space group *Fdd*2.

The lattice vectors (201), (021) and (001), when applied to the triclinic unit cell, lead to a face-centered cell with $a = 30.066$, $b = 21.937$, $c = 4.098$ Å, $\alpha = 89.87$, $\beta = 89.69$, $\gamma = 90.21^\circ$, Z = 8. While the deviations of these angles from 90° are somewhat greater than the reported precision estimates of ~0.07° (Zyuzin *et al.*, 1997), they are not out of line with the *accuracies* that are often encountered (Taylor & Kennard, 1986; Marsh, 1995). Proof of the higher symmetry lies in the atom coordinates: after transformation and translation to an appropriate origin, they can be averaged according to the symmetry of *Fdd*2 within r.m.s. (root mean square) deviations of less than 0.01 Å. The revised coordinates are given in Table 1.

Perhaps a word of caution is in order: there may be danger in assuming that the symmetry of a reported structure should be revised without access to the basic experimental data. However, the danger seems minimal in the present case, where the reported structure conforms to the higher symmetry within such small deviations; since the structure obeys the symmetry of *Fdd*2 (Laue group, *mmm*), the original data must do the same. Where examination of the original data – particularly the very weak reflections – may be vitally important is in cases involving the ambiguity between a centrosymmetric and a noncentrosymmetric structure within the same Laue group, since seemingly important distortions from centrosymmetry may be reflected in only minimal changes in all but the very weakest diffraction intensities.

Table 1
Fractional atomic coordinates, in space group *Fdd*2.

	x	*y*	*z*
O1	0.240	0.3017	0.2488
O2	0.2332	0.3967	0.5573
N1	0.2799	0.3243	0.3771
N2	0.2707	0.3735	0.5314
C1	1/4	1/4	0.0539
C2	0.3090	0.4034	0.6833
C3	0.3024	0.4607	0.8063
C4	0.3377	0.4904	0.9520
C5	0.3787	0.4622	0.9741
C6	0.3842	0.4045	0.8505
C7	0.3496	0.3745	0.7053

I am grateful to Dr Spek, who has developed a program (*PLATON*/*ADDSYM*) which can quickly survey entries in the CSD in search of possible additional symmetry. (The basic program *PLATON* can be accessed at: http://www.cryst.chem.uu.nl/platon.)

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