ADDENDA AND ERRATA

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N,*N*′,*N*″-Trimethyl-*N*,*N*′,*N*″-tris(3-methylphenyl)-1,3,5-benzenetricarboxamide is cubic (space group *Pa*$\bar{3}$) and not orthorhombic (space group *Pbca*). Erratum

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Abstract

N,*N*′,*N*″-Trimethyl-*N*,*N*′,*N*″-tris(3-methylphenyl)-1,3,5-benzenetricarboxamide, $C_{33}H_{33}N_3O_3$, is cubic (space group *Pa*$\bar{3}$) and not orthorhombic (space group *Pbca*) as reported [Azumaya, Kagechika, Yamaguchi & Shudo (1995). *Tetrahedron*, **51**, 5277–5290].

Comment

N,*N*′,*N*″-Trimethyl-*N*,*N*′,*N*″-tris(3-methylphenyl)-1,3,5-benzenetricarboxamide has been reported to crystallize in an orthorhombic cell [a = 17.862 (1), b = 17.863 (1), c = 17.816 (1) Å, Z = 8, space group *Pbca* (No. 61), R = 0.067, refinement on F^2; Azumaya *et al.*, 1995]. The structure factors measured in the orthorhombic cell (kindly supplied by Professor Yamaguchi) conform to the following rule: $|F(hkl)| = |F(klh)| = |F(lhk)|$; $|F(hkl)| \neq |F(khl)|$, illustrated for hkl = 135 and 315 by the values for the various permutations: 55.79, 55.97, 55.03; 3.34, 3.92, 1.54. The coordinates have been recovered from the Cambridge Structural Database (refcode ZEMKIL; Allen *et al.*, 1991); if the x coordinates are decremented by $\frac{1}{2}$, then the (so-called orthorhombic) coordinates of the triplet of atoms C1/C3/C5 are related as x,y,z, z,x,y and y,z,x, respectively. These are the coordinates of Wyckoff position c (site symmetry 3) of space group *Pa*$\bar{3}$, a supergroup of *Pbca*. This relationship also holds for the triplets of atoms C2/C4/C6, C7/C16/C25, O1/O2/O3, N1/N2/N3, C8/C17/C26, C9/C18/C27, C10/C19/C28, C11/C20/C29, C12/C21/C30, C13/C22/C31, C14/C23/C32, C15/C24/C33, H1/H2/H3, H4/H14/H24, H5/H15/H25, H6/H16/H26, H7/H17/H27, H8/H18/H28, H9/H19/H29, H10/H20/H30, H11/H23/H33, H12/H21/H31 and H13/H22/H32. The symmetrized coordinates have been deposited with the Cambridge Structural Database. The sample s.u.'s (for the triplets) are always very close to the values quoted for the experimental s.u.'s, except for the last three hydrogen triplets, where it is clear that atoms H11, H12 and H13 have been somewhat misplaced. In principle, further refinement is not needed as both space groups are centrosymmetric (Schomaker & Marsh, 1979; Marsh, 1995). The above relationships illustrate a point made often in the past, *e.g.* that 'the true symmetry of the lattice is determined far more reliably by the symmetry of the entire structure than by cell dimensions obtained from the setting angles of a few fiduciary reflections' (Herbstein & Marsh, 1998).

The October 1997 version of the Cambridge Structural Database (some 175 000 entries) gives 202 hits for space group No. 205, referring to 162 different compounds. For three of these, Z = 24 (*i.e.* no symmetry required), 77 have Z = 8 (symmetry 3) and 76 have Z = 4 (symmetry $\bar{3}$); the discrepancy between 162 and 156 is accounted for by other values of Z.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1189). Services for accessing these data are described at the back of the journal.

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