ADDENDA AND ERRATA

Acta Cryst. (1998). C**54**, 1193

Comment on *Interwoven Hydrogen-Bonding Networks in Benzene-1,3,5-triacetic Acid* by Fitzgerald & Gerkin (1997)

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Abstract

Fitzgerald & Gerkin [*Acta Cryst.* (1997), C**53**, 967–969] reported 'Interwoven Hydrogen-Bonding Networks in Benzene-1,3,5-triacetic Acid'. Within the paper they state that 'the hydrogen bonds involve each molecule in a three-dimensional network'. Re-examination of the structure using the deposited coordinates, however, shows that the hydrogen-bonded networks defined in the original paper are in fact separate two-dimensional layers which are not interwoven. In addition, the structure is perhaps better described in terms of one-dimensional ladder-like chains, with no more than van der Waals interactions between the ladders.

Comment

The recent report by Fitzgerald & Gerkin (1997) of 'Interwoven Hydrogen-Bonding Networks in Benzene-1,3,5-triacetic Acid' contains the statement that 'the hydrogen bonds involve each molecule in a three-dimensional network'. Re-examination of the structure, as part of an ongoing interest in interpenetration of nets in crystal structures (Batten & Robson, 1998), has shown that the networks defined by the hydr gen bonding interactions, as defined by the authors, are in fact two-dimensional layers two molecules thick. These layers are not interwoven, but are separate from each other and stack in the direction of the *c* axis. Adjacent layers are related by an *n* glide. Closer examination of Fig. 2 in the original paper confirms this conclusion.

Moreover, the 'hydrogen bonds' which form the four-membered O_2H_2 rings described in the original paper are extremely long [O···H 2.88 (3) and O···O 3.020 (2) Å, compared to 2.72 and 3.04 Å, respectively, for the sum of the van der Waals radii (Bondi, 1964)], and should probably be regarded as no more than normal van der Waals interactions. Similar reservations (Cotton *et al.*, 1997) have been expressed about a number of C—H···N hydrogen bonds described in the literature. The structure is thus now described in terms of one-dimensional ladder-like chains defined only by the hydrogen bonds of the eight-membered cyclic dimer interactions (Fig. 1). This ladder motif is perhaps one of the simplest that could be envisaged for molecules with this geometry of hydrogen-bonding functionality.

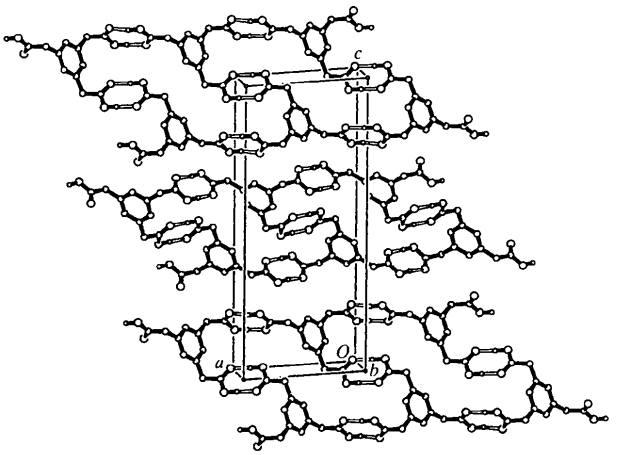

Fig. 1. *ORTEP*III (Burnett & Johnson, 1996) diagram of the one-dimensional ladders in the structure of benzene-1,3,5-triacetic acid. H atoms not involved in hydrogen bonding are omitted for clarity. Circles in order of decreasing size represent O, C and H atoms, and hydrogen bonds are depicted by open bonds.

References

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Response to Batten's (1998) Comment on *Interwoven Hydrogen-Bonding Networks in Benzene-1,3,5-triacetic Acid*

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In response to the comment by Batten [*Acta Cryst.* (1998), C**54**, 1193], we wish to note, to preclude misinterpre-