

ADDENDA AND ERRATA

Acta Cryst. (1998). C54, 1193

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

STUART R. BATTEN

Department of Chemistry, Monash University, Clayton, Victoria 3168, Australia. E-mail: stuart.batten@sci.monash.edu.au

(Received 19 January 1998; accepted 6 March 1998)

Abstract

Fitzgerald & Gerkin [*Acta Cryst.* (1997), C53, 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 hydrogen 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 O₂H₂ 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.

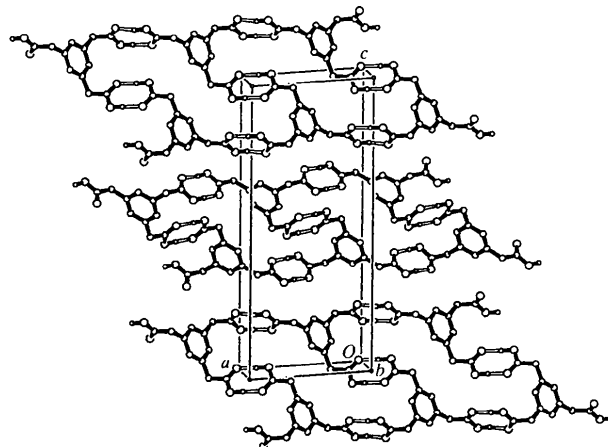


Fig. 1. ORTEP (Burnett & Johnson, 1996) diagram of the one-dimensional ladders in the structure of benzene-1,3,5-triacetic acid. H atoms not involved in hydrogen bonding are omitted for clarity. Circles in order of decreasing size represent O, C and H atoms, and hydrogen bonds are depicted by open bonds.

References

- Batten, S. R. & Robson, R. (1998). *Angew. Chem. Int. Ed. Engl.* **37**. In the press.
 Bondi, A. (1964). *J. Phys. Chem.* **68**, 441–451.
 Burnett, M. N. & Johnson, C. K. (1996). ORTEP. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
 Cotton, F. A., Daniels, L. M., Jordan, G. T. IV & Murillo, C. A. (1997). *Chem. Commun.* pp. 1673–1674.
 Fitzgerald, L. J. & Gerkin, R. E. (1997). *Acta Cryst.* C53, 967–969.

Acta Cryst. (1998). C54, 1193–1194

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

LAWRENCE J. FITZGERALD AND ROGER E. GERKIN

Department of Chemistry, The Ohio State University, Columbus, Ohio 43210, USA. E-mail: rgerkin@magnus.acs.ohio-state.edu

(Received 6 March 1998; accepted 24 March 1998)

In response to the comment by Batten [*Acta Cryst.* (1998), C54, 1193], we wish to note, to preclude misinterpretation,