Table 2. *Distances* (Å), *angles* (°), *hydrogen-bond lengths* (Å) *and torsion angles* (°)

N(1)–C(1)	1·485 (2)	N(1)–C(1)–C(2)	112·2 (1)
C(1)–C(2)	1·514 (2)	C(1)–C(2)–C(3)	111·6 (1)
C(2)–C(3)	1·519 (2)	C(2)–C(3)–C(4)	113·9 (1)
C(3)–C(4)	1·517 (2)	C(3)–C(4)–C(5)	112·3 (1)
C(4)–C(5)	1·519 (2)	C(4)–C(5)–C(6)	114·3 (1)
C(5)–C(6)	1·522 (2)	C(5)–C(6)–C(7)	110·0 (1)
C(6)–C(7)	1·511 (2)	C(6)–C(7)–N(7)	113·6 (1)
C(7)–N(7)	1·485 (2)		
N(1)···Cl(1)	3·193 (2)	N(1)–C(1)–C(2)–C(3)	−178·9 (1)
N(1)···Cl(1^{i})	3·339 (2)	C(1)–C(2)–C(3)–C(4)	172·5 (1)
N(1)···Cl(1^{ii})	3·266 (2)	C(2)–C(3)–C(4)–C(5)	−179·9 (1)
N(1)···Cl(2^{iii})	3·163 (2)	C(3)–C(4)–C(5)–C(6)	175·3 (1)
N(7)···Cl(2)	3·163 (2)	C(4)–C(5)–C(6)–C(7)	−177·5 (1)
N(7)···Cl(2^{iv})	3·174 (2)	C(5)–C(6)–C(7)–N(7)	177·5 (1)
N(7)···Cl(2^{i})	3·123 (2)		

Symmetry code: (i) $1+x, y, z$; (ii) $1-x, 1-y, 1-z$; (iii) $1-x, 1-y, 2-z$; (iv) $1-x, -\frac{1}{2}+y, \frac{3}{2}-z$.

hydrobromide (Brisson & Brisse, 1984), and in both compounds the $C_7H_{20}N_2^{2+}$ cations present a similar curvature (Fig. 1). Unit-cell packing is the same as Fig. 2 in the publication on the dihydrobromide. The cation has an all-*trans* zigzag conformation (Table 2). Although there is an exception (Holmes, Day, Harland, Sau & Holmes, 1984), the all-*trans* structure is the most common for long-chain aliphatic α,ω-diamines and diammonium ions (Borkakoti, Lindley, Moss & Palmer, 1978; McNeil, Scheidt & Thomas, 1981; Oouchi, Takenaka & Sasada, 1986; Binnie & Robertson, 1950; Brown, 1966).

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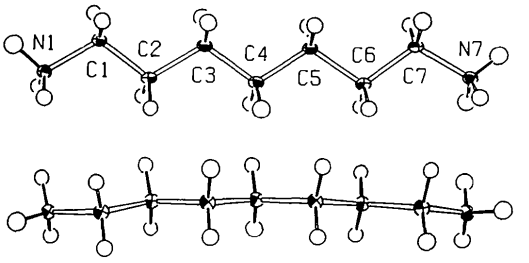

Fig. 1. Two views 90° apart of the 1,7-heptanediyldiammonium cation. The ellipsoids correspond to 50% probability.

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Book Review

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. O. Gould, Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ, Scotland). As far as practicable books will be reviewed in a country different from that of publication.

Acta Cryst. (1988). C**44**, 1153–1154

Crystallographic databases. Edited by F. H. ALLEN, G. BERGERHOFF and R. SIEVERS. Pp. 221. Chester, England: International Union of Crystallography, 1987. Price US$ 20.00. (Paper.)

This book is a collection of articles dealing with methods of crystallographic database compilation and searching, and deals specifically with those crystallographic databases already in existence. It is a useful reference if one wishes to do large-scale analysis of published crystallographic data, or if one needs to provide easy access to crystallographic data as part of a service. The book would also be useful to non-crystallographers as an introduction to the various crystallographic databases that are available.

The articles are divided into four sections, with the first consisting of an overview of crystal structure analysis for the non-specialist, and an introduction to printed crystallographic archives and reference works. The second section is the most interesting to structural scientists as it contains descriptions of the major crystal structure databases. This section contains information on the inclusion criteria, abstraction methods, error checking and availability of the Cambridge Structural Database (CSD), the Inorganic Crystal Structure Database (ICSD), the NRCC metals

crystallographic data file (CRYSMET), and the Protein Data Bank (PDB). There is an additional article detailing some applications and future development plans for the CSD. The article on the PDB has the shortest descriptive section, but the limited size of the database makes it possible to present a list of the current coordinate sets available, and also an example program to read and manipulate a PDB dataset.

The third section describes various non-structural crystallographic databases, the best known of these being the powder diffraction file. Other databases dealt with are the NBS crystal data file, a short piece on the NBS biological macromolecular crystallization database, and the database of order/disorder structures. Of particular interest is the section on the NBS crystal data file, which, while not providing direct access to structural data, appears to be of great use to those providing a crystal structure service who need a comprehensive check for previous crystal structure determinations. Those investigating correlations of physical properties within classes of compounds would also find the comprehensive nature of this database appealing. The final section describes the integrated software systems that exist to access some of the databases described in the previous sections. The most familiar to UK crystallographers is the Chemical Databank System (CDS) based at Daresbury. In the last four years this has been transformed from an alternative interactive access system for the CSD to a system that provides similar interactive interfaces to the three main non-macromolecular crystallographic structure databases, and other databases of interest to the structural scientist. The article on the CDS provides a description of the databases available, a paragraph on the file structure and examples of search technique. A similar system is under development in Canada, with a primary search based around the NBS crystal data file. The article also gives details of plans to integrate the three small structure databases further, with this initial primary search allowing data retrieval from the appropriate database. The article is slightly less useful than the others as it describes an incomplete system. More space is, however, devoted to the mechanics of remote access than in the other articles. A third integrated system exists in Germany based around the software originally developed for the ICSD, and the article dealing with this system gives a short description of the query language, the post-search data processing options available (output formatting and plotting), and details of how the appearance of one integrated structure database is created from the three small structure databases and the NBS crystal data file.

This book provides a great deal of information about the various crystallographic databases available. To use any of the systems described would require further reading of the documentation for that system, but this book gives a good overview of the various styles of query language used, points one in the direction of the correct database to use, and is a useful sourcebook for those interested in accessing the large pool of crystallographic results.

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