

study is part of a systematic evaluation of the distortion of structural groups due to hydrogen bonding.

Crystal-structure data used in the study are taken from neutron diffraction analyses in the literature and part of the data was retrieved with the *TOOL-IR* system (Yamamoto, Negishi, Ushimaru, Tozawa, Okabe & Fujiwara, 1975). The relevant parameters were recalculated with *UNICS* (1967) if they and their estimated standard deviations were not specified. Values uncorrected for thermal motion were used. Data were included in this study only if the e.s.d.'s of all the relevant lengths were equal to or less than 0.010 Å and the O...O hydrogen-bond length was less than 2.7 Å. Carboxyl groups connected by a symmetric hydrogen bond were excluded from the data because the 'structure' and nature of the symmetric hydrogen bond are still not completely understood (Catti & Ferraris, 1976; Olovsson & Jönsson, 1976; Ichikawa, 1978).

### Results and discussion

The relevant parameters are given in Table 1. As shown in Fig. 1, there is a correlation between the C—O and O—H lengths: C—O decreases linearly with increasing O—H (*i.e.* decreasing O...O), both being in a competitive relationship. It can be estimated from Fig. 1 that the C—O length shortens by about 0.035 Å when the O—H length increases from its nonhydrogen-bonded value of 0.96 Å to about 1.20 Å when

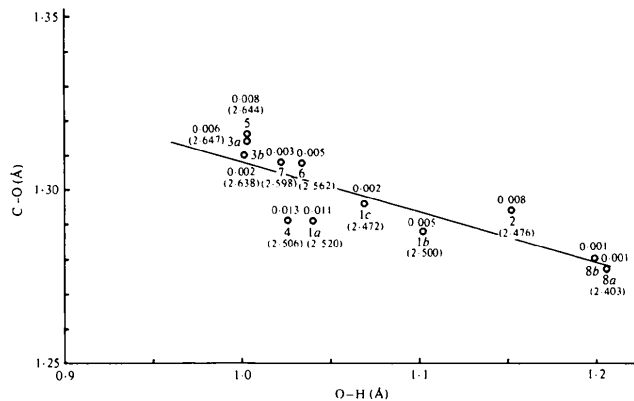


Fig. 1. Diagram of the correlation between C—O and O—H distances in hydrogen-bonded carboxyl groups. The straight line is the least-squares fit of data points. The number of compounds and the deviations of each point from the line are given together with the O...O distances in parentheses.

*Acta Cryst.* (1979). **B35**, 1301

**Crystal and molecular structure of a sympathomimetic amine, tyramine hydrochloride.** BY ALOKA PODDER, J. K. DATTAGUPTA and N. N. SAHA, *Crystallography and Molecular Biology Division, Saha Institute of Nuclear Physics, Calcutta 700009, India* and W. SAENGER, *Max-Planck-Institut für Experimentelle Medizin, Abteilung Chemie, D-3400 Göttingen, Federal Republic of Germany*

(Received 28 March 1979)

### Abstract

A printer's error is corrected. In Table 1 of the paper by Podder, Dattagupta, Saha & Saenger [*Acta Cryst.* (1979), **B35**, 649–652] the value for *b* should be 10.768 (2) Å.

0567-7408/79/051301-01\$01.00

forming a strong hydrogen bond. On the other hand, no correlation could be found between C—O—H angle and O—H length: the C—O—H angles are randomly distributed over 109.4 ~ 114.4° with a mean value of 112.2° (Table 1).

The author thanks the Hokkaido University Computing Centre and the Computing Centre of the University of Tokyo for the use of the FACOM 230-60/75 and HITAC 8800/8700 computers respectively.

### References

- ALBERTSSON, J. & GRENTHE, I. (1973). *Acta Cryst.* **B29**, 2751–2760.  
 CATTI, M. & FERRARIS, G. (1976). *Acta Cryst.* **B32**, 2754–2756.  
 CURRIE, M., SPEAKMAN, J. C. & CURRY, N. A. (1967). *J. Chem. Soc. A*, pp. 1862–1869.  
 ELLISON, R. D., JOHNSON, C. K. & LEVY, H. A. (1971). *Acta Cryst.* **B27**, 333–344.  
 ELLISON, R. D. & LEVY, H. A. (1965). *Acta Cryst.* **19**, 260–268.  
 HAMILTON, W. C. & IBERS, J. A. (1968). *Hydrogen Bonding in Solids*. New York: Benjamin.  
 ICHIKAWA, M. (1978). *Acta Cryst.* **B34**, 2074–2080.  
 ICHIKAWA, M. (1979). To be published.  
 KOETZLE, T. F., HAMILTON, W. C. & PARTHASARATHY, R. (1972). *Acta Cryst.* **B28**, 2083–2089.  
 MACKAY, M. F. (1975). *Cryst. Struct. Commun.* **4**, 225–228.  
 NAKAMOTO, K., MARGOSHES, M. & RUNDLE, R. E. (1955). *J. Am. Chem. Soc.* **77**, 6480–6486.  
 OLOVSSON, I. & JÖNSSON, P.-G. (1976). *The Hydrogen Bond*, Vol. II, ch. 8, edited by P. SCHUSTER, G. ZUNDEL & C. SANDORFY. Amsterdam: North-Holland.  
 SABINE, T. M., COX, G. W. & CRAVEN, B. M. (1969). *Acta Cryst.* **B25**, 2437–2441.  
 UNICS (1967). *Universal Crystallographic Computing System*, edited by T. SAKURAI. Crystallographic Society of Japan.  
 VILMINOT, S. & PHILIPPOT, E. (1976). *Acta Cryst.* **B32**, 1817–1822.  
 YAMAMOTO, T., NEGISHI, M., USHIMARU, M., TOZAWA, Y., OKABE, K. & FUJIWARA, S. (1975). Proc. 2nd USA-Jpn Comput. Conf. pp. 159–165.

All the relevant information is contained in the *Abstract*.

© 1979 International Union of Crystallography