unweighted and weighted residuals $R = 0{\cdot}036$ and $wR = 0{\cdot}042$. $S = 2{\cdot}03$. The conventional R for all reflections including unobserved ones was 0·052. Maximum and minimum peak heights in the final difference synthesis were 0·41 and −0·30 e Å^{-3}. $(\Delta/\sigma)_{\max} = 0{\cdot}004$. All calculations were performed on a VAX computer using *SDP/VAX* (Frenz, 1978). Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Table 1* gives the atomic coordinates and thermal parameters. Selected bond distances and bond angles are listed in Table 2. Fig. 1 shows the complex (1–2), Figs. 2 and 3 show projections of the crystal structure (Keller, 1988; Johnson, 1976).

Financial support by Deutsche Forschungsgemeinschaft, Fonds der Chemischen Industrie, Stiftung Volkswagenwerk, BASF AG and JCPDS/International Centre for Diffraction Data is gratefully acknowledged.

References

Ferraris, J. P., Poehler, T. O., Bloch, A. N. & Cowan, D. O. (1973). *Tetrahedron Lett.* **27**, 2553–2556.

Frenz, B. A. (1978). *The Enraf-Nonius CAD-4 SDP-A Real-Time System of Concurrent X-ray Data Collection and Crystal Structure Solution.* In *Computing in Crystallography*, edited by H. Schenk, R. Olthof-Hazekamp, H. van Koningsveld & G. C. Bassi, pp. 64–71. Delft Univ. Press.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Kachkurova, I. Ya, Ashkinadze, L. D., Shamsutdinova, M. Kh. & Kazitsyna, L. A. (1987). *Zh. Org. Khim.* **23**, 1629–1634.

Keller, E. (1988). *SCHAKAL*88. *A Fortran Program for the Graphical Representation of Molecular and Crystallographic Models.* Albert-Ludwigs-Univ., Freiburg, Germany.

---

* Tables of anisotropic displacement factors and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53747 (22 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

SHORT COMMUNICATION

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1991). C**47**, 1131–1132

Structure of the complex of imidazole and picric acid. Corrigendum and addendum.

By Frank H. Herbstein and Moshe Kapon, *Department of Chemistry, Technion – Israel Institute of Technology, Haifa, Israel* 32000

(*Received* 17 *October* 1990; *accepted* 19 *November* 1990)

Abstract

The crystallographic results of Soriano-García, Schatz-Levine, Toscano & Iribe [*Acta Cryst.* (1990), C**46**, 1556–1558] show unequivocally that this substance is the salt ‘imidazolium picrate’ and not a complex of some kind between the neutral moieties ‘imidazole’ and ‘picric acid’.

This crystal structure was reported (Soriano-García, Schatz-Levine, Toscano & Iribe, 1990) under the title given above. However, the authors state “The imidazole ring is protonated and makes a dihedral angle of 112·6 (1)° with the six-membered ring of picric acid.” This provides clear evidence for classifying the material as the salt, imidazolium picrate.

We have computed the *ORTEP* stereodiagram (Fig. 1; Johnson, 1965). The moieties are arranged in zigzag ribbons, with axes along [100]; each ‘picrate’ oxygen is hydrogen bonded to the two N—H groups of the imidazolium cation, the N(1)···O(1)···N(3) angle being 77·6 (4)°. Despite slight asymmetry in the hydrogen bonding $\{d[\mathrm{N(1)\cdots O(1)}] = 2{\cdot}710\,(4)$ and $d[\mathrm{N(3)\cdots O(1)}] = 2{\cdot}825\,(5)$ Å$\}$, the imidazolium cation does not deviate significantly from *mm*2 symmetry, in contrast to the situation in the neutral molecule (Craven, McMullan, Bell & Freeman, 1977). The mutual disposition of the ring planes of the components is such that π–π^* interaction is impossible; the moiety dimensions and the location of the H atoms show that this is not a hydrogen-bonded complex of neutral molecules, as in imidazole–5,5-diethylbarbituric acid (Hsu & Craven, 1974). Thus the material is not a ‘complex’ in any of the (here relevant) senses in which this term is abused (le Noble, 1974).

Somewhat similar confusions of nomenclature occur in the report of the crystal structure of pyridinium picrate (Talukdar & Chaudhuri, 1976).

0108-2701/91/051131-02$03.00

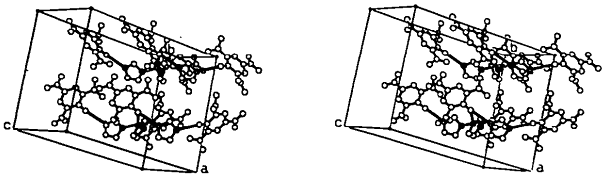

Fig. 1. *ORTEP* stereodiagram of the hydrogen-bonding arrangement in the crystal structure of imidazolium picrate. The atoms are shown as spheres with arbitrary radii of 0·2 Å; the N atoms have principal circles, with N(3) differentiated by hatching. H atoms were omitted for clarity. Hydrogen bonds are shown by thicker lines.

References

Craven, B. M., McMullan, R. K., Bell, J. D. & Freeman, H. C. (1977). *Acta Cryst.* **B33**, 2585–2589.

Hsu, I.-N. & Craven, B. M. (1974). *Acta Cryst.* **B30**, 988–993.

Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

Noble, W. J. le (1974). *Highlights of Organic Chemistry, An Advanced Textbook*, ch. 23, pp. 841–842. New York: Dekker.

Soriano-García, M., Schatz-Levine, M., Toscano, R. A. & Iribe, R. V. (1990). *Acta Cryst.* **C46**, 1556–1558.

Talukdar, A. N. & Chaudhuri, B. (1976). *Acta Cryst.* **B32**, 803–808.