(De Ranter & Van Dijck, 1971). The essence of the following conclusions is independent of the choice of the parameters in Table 1.

The experimental valence ($3s^23p^6$) charge densities of KCl at 300 K along the three principal directions are shown in Figs. 1 and 2. The experimental structure factors and Debye–Waller coefficients are from Patomäki & Linkoaho (1969). Figs. 1 and 2 clearly demonstrate the differences between the electron densities around the positive and negative isoelectronic ions; the latter are more diffuse. Some very slight aspherical deformations seen in Figs. 1 and 2 are probably insignificant. The effect on the charge densities from the one-term Gaussian approximation has been estimated by the differences between the core structure factors mentioned above. This effect appeared to be of the same order or smaller than the influence of experimental errors ($\leq 0{\cdot}04$ e Å^{-3} in Figs. 1 and 2). The error estimates shown by vertical bars in Figs. 1 and 2 roughly indicate both the effect of experimental errors and the effect due to the Gaussian approximation. (Possible error from inaccuracy of the scale factor is omitted.)

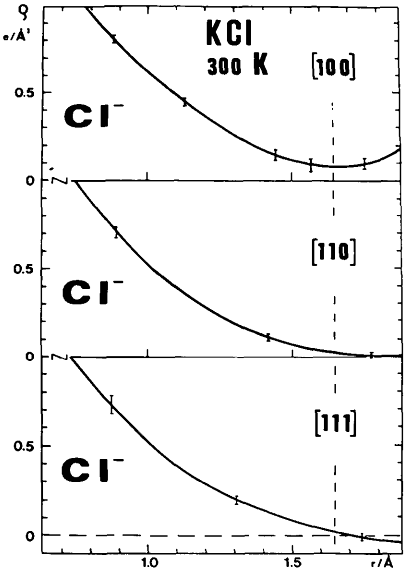

Fig. 2. The valence-electron charge density in the vicinity of the Cl⁻ ion along the [100], [110] and [111] directions for KCl at 300 K. The distance where the density between nearest neighbours reaches its minimum value is indicated by vertical broken lines.

In the light of the preceding considerations, the one-term Gaussian method which is used to subtract the core-electron contribution and to obtain the experimental valence charge densities seems satisfactory. The calculations are simple and the accuracy good enough compared with the effect of experimental errors. It is possible to attain still better accuracy by decreasing the limiting value r_c^* somewhat, say about 10%. By making this small reduction, one does not lose information on the valence charge distribution. The thermal smearing function is needed only for core electrons, where the use of isotropic approximation (Debye–Waller coefficients) is better justified. The refinement of the method by including symmetry-adapted aspherical thermal vibrations of core electrons is, however, quite straightforward.

References

Bagus, P. S. (1965). *Phys. Rev.* **139**, A619–A634.
De Ranter, C. J. & Van Dijck, M. (1971). *Z. Kristallogr.* **134**, 97–106.
Linkoaho, M. V. (1972). *Phys. Scr.* **5**, 271–272.
Linkoaho, M. V. H. (1979). *Acta Cryst.* A**35**, 140–142.
Patomäki, L. K. & Linkoaho, M. V. (1969). *Acta Cryst.* A**25**, 304–305.

Acta Cryst. (1980). A**36**, 156

The qualitative and quantitative analysis of renal stones by X-ray diffraction and electron-probe techniques.

By Monte Modlin, *Research Project Supervisor, Department of Urology, Medical School, Observatory 7925, Cape Town, Republic of South Africa*

(*Received* 7 *August* 1979; *accepted* 1 *September* 1979)

Abstract

The *Abstract* by Modlin & Rodgers [Acta Cryst. (1978), A**34**, S4, 381] was submitted without the knowledge of the present author, who was not aware of its content. Only preliminary discussions and work on certain aspects of a research programme had taken place at the time that the *Abstract* was submitted. The conclusions claimed in the last sentence had not been arrived at.

All relevant information is contained in the *Abstract*.

0567-7394/80/010156-01$01.00