tions, the phase I transition was shifted to temperatures above 125 °C.

Discussion

Brown & McLaren (1962) measured the proton magnetic resonance line widths of polycrystalline ammonium nitrate and explained the low values due to 'nil' intra-NH_4 contribution which they interpreted as evidence of free rotation of the NH_4^+ ion. The libration amplitudes of the hydrogens obtained by Choi et al. (1972) from neutron diffraction also suggest a nearly free rotation producing spherical symmetry for the cation. As in alkali nitrates, the foreign cations may thus be expected to enter the lattice substitutionally.

In phases IV and II, steric hindrance prevents any large amplitude oscillation of the nitrate ion. On the other hand, in phase I (Shinnaka, 1959), X-ray studies provide evidence for hindered rotation of the nitrates. The absence of phase II in crystals containing K^+ ions is traceable to the onset of rotational disorder of the NO_3^- ions, when they have the symmetry of phase II. The cation–oxygen distance in phase II, ~ 3.0 Å, is larger than the maximum K–O distance (for eightfold coordination in the phase II structure) (International Tables for X-ray Crystallography, 1968), 2.98 Å. This is found to be true in trigonal phase I of potassium nitrate (Tahvonen, 1949), where anion rotation is present for the K–O distance 2.96 Å for sixfold coordination (max. K–O distance 2.91 Å). The rotation stops when the distance

decreases to 2.88 Å (Shinnaka, 1962) in trigonal phase III. Likewise, the delayed onset of phase I in crystals containing Cs^+ ions, is due to the Cs–O distances varying from 3.0–3.59 Å (International Tables for X-ray Crystallography, 1968).

The author desires to thank Dr S. Swaminathan and Professor C. Ramasastry for their interest in this work.

References

AMOROS, J. L., ARESSE, C. & CANUT, M. (1962). Z. Kristallogr. 117, 92–107.
BROWN, R. N. & MCLAREN, A. C. (1962). Proc. Roy. Soc. A266, 329–343.
CHOI, G. S., MAPES, J. E. & PRINCE, E. (1972). Acta Cryst. B28, 1357–1361.
COATES, R. V. & CREWE, J. M. (1961). Nature, Lond. 190, 1190.
HENDRICKS, S. B., POSNJAK, E. & KRACEK, F. C. (1932). J. Amer. Chem. Soc. 54, 2766–2786.
International Tables for X-ray Crystallography (1968). Vol. III, pp. 258–259. Birmingham: Kynoch Press.
SALHOTRA, P. P., SUBBA RAO, E. C. & VENKATESWARLU, P. (1969). J. Phys. Soc. Japan, 27, 621–629.
SHINNAKA, Y. (1959). J. Phys. Soc. Japan, 14, 1073–1080.
SHINNAKA, Y. (1962). J. Phys. Soc. Japan, 17, 820–828.
TAHVONEN, P. E. (1949). Ann. Acad. Sci. Fenn. A42, 20–44.
YANAGI, T. (1965). J. Phys. Soc. Japan, 20, 1351–1365.

The computation of radial distribution functions for glassy materials. Errata.

By J. H. KONNERT and J. KARLE, Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, D. C. 20375, U.S.A.

Corrections are given to equations (5), (6), (8) and (15) in the paper by Konnert & Karle [Acta Cryst. (1973). A29, 702–710].

In a previous paper of the above title (Konnert & Karle, 1973), the term $2r/\pi$ on the right-hand side of equation (5) should be replaced by $r/[(2\pi)^{1/2}]$ and l_{ij}^{-1} should be inserted after the summation sign, the right-hand sides of equations (6) and (8) should be multiplied by Δs and $(\Delta s)^2$ respectively, and the term ϱ_0 in equation (15) should be replaced by $4\pi r\varrho_0$. The symbol Δs represents the interval between successive points in the summation.

Reference

KONNERT, J. H. & KARLE, J. (1973). Acta Cryst. A29, 702–710.