TABLE III. Calculation of the parameters in the semiempirical equation of state of sodium[a]

Atomic volume Ω_0[b]	37.8
Ionization potential[c]	1.81
Heat of sublimation[d]	8.23
$-E_c$	10.04
ΩB_0[e]	2.74
A (empirical)	2.29
B (empirical)	5.46
B (theoretical)	3.11
C (empirical)	17.79
C (theoretical)	16.6
$-\Omega dB/d\ln\Omega$ (empirical)	8.73
$-\Omega dB/d\ln\Omega$ (experimental)	8.80

[a] All entries except the atomic volume are in units of 10^{-12} erg atom^{-1}, Ω_0 is in units of 10^{-24} cm^3 atom^{-1}.
[b] From x-ray data corrected using S. L. Quimby and S. Siegel thermal expansion data, Phys. Rev. 54, 76 (1938).
[c] F. Seitz, see reference 19.
[d] *American Institute of Physics Handbook* (McGraw-Hill Book Company Inc., New York, 1957).
[e] B_0 at 4.2°K from C. A. Swenson, Phys. Rev. 99, 423 (1955).

In addition, the experimental value of $\Omega dB/d\ln\Omega$ is given to compare with the value calculated from the equation of state. The atomic volume at 0°K is also given in Table III.

B (empirical) and B (theoretical) do not agree especially well, at least in part due to the structure of the equations, a small error in the bulk modulus results in large errors in B. The values of C(emp) and C(theo) agree quite well, the empirical value of $\Omega dB/d\ln\Omega$ is surprisingly near the experimental value. One would have expected the breakdown of the assumptions regarding the Frohlich-Bardeen equation of state to have yielded an empirical value appreciably less than the experimental value.[22]

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Crystal Structure of Ferroelectric $LiH_3(SeO_3)_2$*

K. VEDAM, Y. OKAYA, AND R. PEPINSKY
Crystal Research Laboratory, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania

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The structure of the room-temperature ferroelectric $LiH_3(SeO_3)_2$ has been determined by x-rays, using the heavy-atom method, and refined on the IBM 704. The crystals are monoclinic, with space group Pn and $a=6.25_8$ A, $b=7.88_6$ A, $c=5.43_3$ A, $\beta=105.2°$. Fairly strong O−H···O bonds with distances 2.52, 2.56, and 2.57 A are found, nearly perpendicular to the polar direction. The O−Se−O angles in one of the two selenite ions are rather similar; in the other ion these angles are unequal, as in the structure of H_2SeO_3. Possible positions for the Li ions are given based on crystal-chemical considerations.

I. INTRODUCTION

FERROELECTRICITY is observed in lithium trihydrogen selenite, $LiH_3(SeO_3)_2$, over the temperature range from −196°C to 90°C.[1] The spontaneous polarization is the largest yet observed in a water-soluble crystal: 15 μcoul/cm^2. The coercive field, 1400 volts/cm, is disadvantageously high when compared to that of $(glycine)_3\cdot H_2SO_4$: 220 volts/cm.[2]

A recent structure analysis of $(glycine)_3\cdot H_2SO_4$, utilizing both x-ray[3] and neutron[4] diffraction and the x-ray anomalous dispersion method[5–7] for establishment of the absolute configuration of the polar crystal, has permitted assignment of a polarization and switching mechanism for that ferroelectric.

The x-ray analysis reported here is a first step in the development of similar understanding of the polarization and switching mechanism in $LiH_3(SeO_3)_2$. No attempt has been made in this study to locate hydrogen atoms, which would be very difficult if not impossible in the presence of the heavy selenium atom. A neutron analysis at the Brookhaven reactor, and an anomalous dispersion study similar to that accomplished for $(glycine)_3\cdot H_2SO_4$, are in progress.

II. EXPERIMENTAL

The crystals of $LiH_3(SeO_3)_2$ used in the present x-ray study were grown from aqueous solution of lithium hydroxide or lithium carbonate and selenious acid in stoichiometric ratios. These crystallize in the monoclinic system, with space group Pn and cell dimensions

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