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Coherent neutron scattering amplitudes of Br and ^{127}I.*

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Neutron diffraction data of KBr and KI yielded the thermal neutron coherent scattering amplitudes in 10^{-12} cm, $b(\mathrm{Br})=0{\cdot}670\pm0{\cdot}004$, $b(^{127}\mathrm{I})=0{\cdot}525\pm0{\cdot}004$, taking $b(\mathrm{K})=0{\cdot}370\pm0{\cdot}001$ as standard.

Neutron powder diffraction measurements of KBr and KI yielded the coherent neutron scattering amplitudes in ratios $b(\mathrm{Br})/b(\mathrm{K})=1{\cdot}81\pm0{\cdot}01$ and $b(^{127}\mathrm{I})/b(\mathrm{K})=1{\cdot}42\pm0{\cdot}01$ respectively. Uncertainties quoted are standard deviations. The pioneer research of Shull & Wollan (1951) gave $b(\mathrm{K})=0{\cdot}35$, $b(\mathrm{Br})=0{\cdot}67$ and $b(^{127}\mathrm{I})=0{\cdot}52$, all in 10^{-12} cm. Recently, Koester & Knopf (1972) obtained $b(\mathrm{K})=0{\cdot}371$, $b(\mathrm{Br})=0{\cdot}677$ and $b(\mathrm{I})=0{\cdot}528$, all with $\pm0{\cdot}002$. Brown & Walker (1966) reported $b(\mathrm{K})=0{\cdot}370\pm0{\cdot}004$, and Bacon & Plant (1968) obtained $b(\mathrm{K})=0{\cdot}369\pm0{\cdot}003$. The agreement among the last three $b(\mathrm{K})$'s is excellent and the weighted average is $b(\mathrm{K})=0{\cdot}370\pm0{\cdot}001$. Using this $b(\mathrm{K})$, our data lead to $b(\mathrm{Br})=0{\cdot}670\pm0{\cdot}004$ and $b(\mathrm{I})=0{\cdot}525\pm0{\cdot}004$. The $b(\mathrm{Br})$ and $b(\mathrm{I})$ values obtained from the Bragg diffraction intensities (Shull & Wollan, and the present work) agree satisfactorily with those deduced from the Christiansen-filter small-angle scattering (Koester & Knopf, 1972). The weighted averages are $b(\mathrm{Br})=0{\cdot}676\pm0{\cdot}001$ and $b(\mathrm{I})=0{\cdot}527\pm0{\cdot}001$, both of which may now be considered as the firmly established amplitude values.

Our samples are Johnson Matthey's spectrographically certified KI, Fisher certified KI and KBr, and Harshaw Optical KI and KBr crystals. These were ground down to <200 mesh in particle size and were dried in air at 150°C for several hours. The powder was then packed into a thin-walled null-matrix Ti–Zr holder 1 cm in diameter. The diffraction data were taken with 1·069 Å at 23°C. The higher-order wavelength contamination is less than 0·04%. Some samples gave weak extraneous peaks or abnormal diffuse scattering other than the intrinsic thermal scattering (Chipman & Paskin, 1959; Iveronova, Parogtopa & Zvyagina, 1967; Kashiwase, 1968). These samples were discarded. At least six independent measurements were made on each reflection. The graphical plotting, log F_{obs} *vs.* $(\sin\theta/\lambda)^2$, was made on the isolated all-even reflections, 200, 220, 222, 400, 422, 440 and 620. The overlapped peak groups are {331, 420} and {531, 600, 442}. These were resolved using the Gaussian profile analysis. The odd-reflection plotting was then made using 111, 311, 331, 511, 333 and 531. The linear least-squares method was then applied to each set of scanning data with and without appropriate weighting factors. The statistical averages of the resultant parameters were employed in the scattering amplitude determination. The Debye–Waller coefficients in Å^{-2} are $B(\mathrm{K})=2{\cdot}6\pm0{\cdot}2$ and $B(\mathrm{Br})=2{\cdot}5\pm0{\cdot}2$ for KBr and $B(\mathrm{K})=3{\cdot}4\pm0{\cdot}3$ and $B(\mathrm{I})=2{\cdot}7\pm0{\cdot}2$ for KI. Wasastjerna (1946) obtained $B(\mathrm{K})=2{\cdot}06$ $B(\mathrm{Br})=1{\cdot}92$ for KBr and $B(\mathrm{K})=2{\cdot}69$ and $B(\mathrm{I})=2{\cdot}37$ for KI at 293°K, some of which are significantly different from our values. The following B values are insignificantly different from ours: $B(\mathrm{K})=2{\cdot}45$ and $B(\mathrm{Br})=2{\cdot}23$ for KBr at 300°K (Meisalo & Inkinen, 1967); $B(\mathrm{K})=3{\cdot}66$ and $B(\mathrm{I})=2{\cdot}92$ for KI at 296°K (Pearman & Tompson, 1967).

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Anomalous neutron scattering and the question of ferroelectricity in $^6Li(N_2H_5)SO_4$.

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The mechanism of the supposed ferroelectric switching in crystals of $Li(N_2H_5)SO_4$ was examined by studying the effect of the anomalous scattering of neutrons from ^{6}Li on the structure factors of Bijvoet pairs both before and after ferroelectric switching. The absence of any observable change confirms the results of Schmidt, Drumheller & Howell [*Phys. Rev.* (1971). B**12**, 4582] that $Li(N_2H_5)SO_4$ is not ferroelectric.

Introduction

The apparent ferroelectric nature of lithium hydrazinium sulphate, $Li(N_2H_5)SO_4$, was reported by Pepinsky, Vedam, Okaya & Hoshino (1958). They observed good hysteresis loops from about −15 to 80°C, although they could find neither a dielectric peak between −196 and 140°C nor a specific heat anomaly between −120 and 205°C.

The crystal structure has been investigated by X-ray diffraction (Niizeki & Koizumi, 1964; Brown, 1964; and