not really revealed strong evidence regarding the mechanism of polarization reversal. Lingafelter *et al.* claim that they have given a mechanism. While they speculate on the geometrics, no physical basis is given.

How, for example, can an electric field perpendicular to the plane of a guanidinium ion cause it to rotate? Further, it is required that one of two equivalent guanidinium ions rotate and become equivalent to the unique one, while the other (of the originally equivalent pair) becomes unique.

I have discussed these points with R. P. Futrelle and W. F. Hall of our laboratory. It is possible that rotations could take place. For example, suppose the groups above and below the guanidinium ions carry negative charges. The guanidinium ion carries a positive charge distributed with threefold symmetry in its plane. It is closer to one negative group than to the other and is in its equilibrium position. Imposition of an electric field strong enough to move these negatively charged groups might move the group which was originally further from the guanidinium ion closer to it, and the one that was closer, further from it. Thus the new equilibrium position could involve a rotation of the guanidinium ion. This much (though not given by Lingafelter *et al.*) is acceptable.

However, it is required that one of two equivalent guanidinium ions rotate. It may be argued that as soon as one of these rotates, all others in the *same* aspect rotate, while the remainder stay essentially in their original positions. Such an argument does not appear to be tenable. It would seem that the probability for rotation would be equal for the two equivalent guanidinium ions (and there does not seem to be any obvious qualitative reason that the unique one should not rotate also). This implies, then, that the *original* GASH crystal should be multiply-twinned, that is, that domains should be present with each of the possible sets of orientations.

Consideration of this possibility leads to the conclusion that the (+, +) and (+, −) (see Geller & Katz, 1962) guanidinium ion configurations should be equally probable. Our calculations (Geller & Katz, 1962), to some extent, included a check of this hypothesis. The (+, −) configuration was preferred. As we have pointed out (Geller & Katz, 1962), the exact (+, +) configuration makes no contribution to intensities of reflections $hk\,.\,l$ with $h-k\neq 3n$. However, because both configurations are equally probable, it is unlikely that the preferred one would have been the (+, −) one (almost exactly) if such disorder actually existed in the crystal. In fact, we also checked a configuration in which the two equivalent guanidinium ions were rotated 30° from their positions given in our Table IV; the calculations showed that these were unlikely. Thus the suggestion made by Lingafelter *et al.* with regard to the polarization reversal lacks a firm foundation.

Unfortunately, despite the publication of a number of papers on GASH, there is little evidence regarding the switching mechanism. Holden, Merz, Remeika & Matthias (1955) pointed out that while they obtained no details regarding it, they did obtain some evidence (which they gave) that it is principally the same as for $BaTiO_3$, that is, 'mainly a nucleation problem of domains'. However, as far as I know, no further evidence substantiating this conclusion has been published.

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## A measurement of the dispersion correction.

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Recently Chipman & Jennings (1963) were able to measure the dispersion correction $\Delta f'$ in the inert gases Ne, Ar, Kr and Xe by an extrapolation of the absolute scattering factor $f$ to $\sin\theta/\lambda=0$ where $f=Z+\Delta f'$. While it would have been possible to calculate $\Delta f'$ from measured values of the absorption coefficient over all wave lengths, such values were not available in sufficient accuracy for Chipman & Jennings to determine whether their measured values of $\Delta f'$ were correct. In none of the four cases was the dispersion correction more than ~2% of $Z$ at the Mo $K\alpha$ radiation employed. We therefore considered it worthwhile to make an *absolute* determination of $\Delta f'$ in a case where the contribution is considerably greater than 2%.

The measurements were made by comparing the ratio in reflection of the 440 scattering factor at Ge $K\beta$ of a perfect crystal of germanium to the 440 scattering factor of a perfect crystal of silicon, both crystals having been previously measured on an absolute basis (DeMarco & Weiss, 1965) at Mo $K\alpha$ where $\Delta f'$ is small. At Ge $K\beta$ ($\lambda=1{\cdot}129$ Å, $\lambda/\lambda_K=1{\cdot}011$) $\Delta f'$ comprises over 30% of the total scattering factor for the 440 in Ge but only ~1½% to the 440 in silicon. A theoretical value of $\Delta f'=+0{\cdot}1$ was employed for silicon, an error of ~50% in $\Delta f'$ only contributing an uncertainty of ¾%.

A Norelco fluorescence unit was employed to produce the Ge $K\beta$ by fluorescence of germanium. Under identical conditions the integrated reflecting power was made of the Si 440 and Ge 440 reflections over a sufficiently large angular range ($\Delta 2\theta=6°$) to ensure that the entire $K\beta$ was diffracted. The thermal diffuse scattering correction was made as in the previous absolute measurements with Mo $K\alpha$. By making several runs and interchanging crystals the beam power appeared constant within the statistical error of ~1½%. The measured value of $\Delta f'$ for Ge $K\beta$ on germanium was determined to be

$$\Delta f'=-4{\cdot}66\pm0{\cdot}3\,.$$

In order to compare this value with theory we employed the values of the oscillator strengths $g$ calculated by Cromer (1965) with the relativistic Dirac–Slater wave functions. We believe these values to be accurate to ~3 % for the $K$ shell. For germanium they give $g_K = 1{\cdot}29$. In addition the previously measured value of the linear absorption coefficient $\mu$ of germanium at Mo $K\alpha$ was employed ($\mu = 325{\cdot}5$ cm$^{-1}$). We believe this value to be accurate to 1 %. The $L$ and $M$ shell contributions to the absorption coefficient and dispersion corrections are small and we have employed the oscillator strengths of Cromer in the procedure suggested by Parratt & Hempstead (1954). The total $L$ and $M$ contribution to the linear absorption coefficient of germanium at Mo $K\alpha$ was taken to be 44 cm$^{-1}$ extrapolated from the measured linear absorption of germanium at Cu $K\alpha$ (352 cm$^{-1}$) believed accurate to ~1½ %. By assuming the wavelength dependence of the absorption coefficient of the $K$ shell to be proportional to $\lambda^{2+\delta}$ we employed the value of $g_K$ calculated by Cromer and the measured value of the absorption coefficient at Mo $K\alpha$ (corrected for $L$ and $M$ shell contribution) to determine $\delta$ from

$$g_K = \frac{\mu_K A(\lambda_K/\lambda)^{2+\delta}}{\pi \varrho a(e^2/mc^2)\lambda_K(1+\delta)} \qquad (1)$$

where $\mu_K$ is the linear absorption coefficient of the $K$ shell at wavelength $\lambda$, $\varrho$ the density, $a$ Avogadro's number, $A$ the atomic weight and $\lambda_K$ the $K$ absorption edge. We obtain $\delta = 0{\cdot}63$ for germanium. The respective $K$, $L$ and $M$ contributions to $\Delta f'$ are thus calculated to be

$$\Delta f' = -4{\cdot}8 \pm 0{\cdot}15(K) + 0{\cdot}21 \pm 0{\cdot}08(L) + 0{\cdot}03 \pm 0{\cdot}02(M) = -4{\cdot}56 \pm 0{\cdot}25\,,$$

in good agreement with the experimental value of $\Delta f' = -4{\cdot}66 \pm 0{\cdot}3$. It appears that even under the best of conditions $\Delta f'$ can only be measured (or calculated) to an error of ~5 %.

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## Cell dimensions and space groups of some olefin–Pt(II) complexes.

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In connection with investigations in our laboratories concerning the stereochemical features of olefin–transition metal complexes, an X-ray analysis of some dihalogenoplatinum compounds was undertaken (Paiaro & Panunzi, 1964, 1965). Besides the determination of conformational parameters such as bond lengths, valence angles and internal rotation angles, the purpose of the work is the assignment of the absolute configuration of the olefin ligand, based upon that of α-phenethylamine (Eliel, 1962), and the correlation of the absolute configuration found with the observed rotations.

Single crystals of:

(I). *trans*-Dichloro(*cis*-2-butene)(*S*)-(α-phenethylamine)Pt(II)
(II). (−)*trans*-Dichloro(*trans*-2-butene)(*S*)-(α-phenethylamine)Pt(II)cyclohexane
(III). (+)*trans*-Dichloro(*trans*-2-butene)(*S*)-(α-phenethylamine)Pt(II)
(IV). (−)*cis*-Dichloro(*trans*-2-butene)(*S*)-(α-phenethylamine)Pt(II)

were obtained by slow crystallization from suitable solvents. Space groups and lattice constants (Table 1) were determined from Weissenberg photographs about the $b$ axis and from precession photographs around the $c$ axis; densities were measured by flotation methods.

Table 1. *X-ray data*

| | Compound | | | |
|---|---|---|---|---|
| Cell constants | (I) | (II) | (III) | (IV) |
| $a$ | 15·64 | 15·59 | 8·87 | 12·55 |
| $b$ | 10·42 | 14·72 | 12·21 | 6·65 |
| $c$ | 9·16 | 9·36 | 6·92 | 8·88 |
| $\beta$ | 90° | 90° | 99° | 102°30′ |
| Space group | $P2_12_12_1$ | $P2_12_12_1$ | $P2_1$ | $P2_1$ |
| $d_{\text{exp}}$ (g.cm$^{-3}$) | 1·98 | 1·62 | 1·99 | 1·99 |
| $d_{\text{RX}}$ | 1·97 | 1·64 | 1·99 | 2·03 |

Complete structure determinations of the compounds (I), (III) and (IV) have been started.

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