fossil fuel burning and low-temperature biological reactions. In high-temperature oxidation Se burns in air to form the white solid SeO_2. The SeO_2 is so readily reduced that even specks of oxidizable dust in the air react with it to form red elemental Se (*10*). On the other hand, S is oxidized to the relatively stable SO_2. Whether the high-temperature process is man-made or is natural, as in volcanic activity, this difference in chemistry between the elements would be manifest.

On the other hand, the low-temperature biological processes produce compounds of S and Se that are volatile. As organic compounds (whose identity is not yet established), Se is volatilized from land plants (*11*). Volatile organic Se compounds are also released in the process of plant degradation (*11*) (possibly as H_2Se). In either case, the very low concentrations in the atmosphere may survive against oxidation long enough to be transported in a similar manner as the gaseous S compounds H_2S and SO_2.

In summary, man initiates the translocation of compounds of S over great distances through fuel combustion, whereas Se is mobilized to a much lesser extent, perhaps owing to the differences in the chemical and physical properties of the tetravalent oxides.

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Hydroxyl Orientation in Muscovite as Indicated by Electrostatic Energy Calculations

Abstract. *The electrostatic energy of the* $2M_1$ *muscovite structure,* $KAl_2(Si_3Al)O_{10}(OH)_2$*, has been calculated as a function of the orientation of the hydroxyl group (O–H distance = 0.97 angstrom). The minimum in the electrostatic energy occurs when the OH bond makes an angle of 18° with the cleavage plane and an angle of 31° with the* b*-axis (in the* a*-*b *plane), which is 2.5° away from the orientation of the transition moment as determined from infrared measurements on single crystals. If the* K^+ *ion is excluded from the calculation, the O–H bond makes an angle of 53° with the cleavage plane. This indicates the strong influence that the interlayer cation exerts on the hydroxyl hydrogen in mica structures.*

The role of the hydroxyl group in micas has recently attracted much attention, particularly in the trioctahedral mica biotite (*1, 2*). Juo and White (*2*) have shown, by examining the pleochroism of the O–H stretching frequencies from oriented biotite films, that the OH orientation depends on the oxidation state of the octahedral iron. The interpretation of the infrared absorption spectra of layer silicates is very complex, and, except for studies of single crystals, one can determine only whether the OH bond is perpendicular to the cleavage plane or inclined. What is needed is a simpler method of determining OH orientation with respect to the other atoms in the crystal structure. Giese *et al.* have shown (*3*) that the hydroxyl hydrogen in diaspore (α-AlOOH) and goethite (α-FeOOH) is found in a position at which the electrostatic energy of the crystal is a minimum, or nearly so. In this report I present evidence that the hydroxyl hydrogen in the mica muscovite, $KAl_2(Si_3Al)O_{10}(OH)_2$, also occupies such a position.

The electrostatic energy of an ionic crystal can be calculated from (*4*)

$$\Phi_0 = -\frac{e^2}{2}\sum_{s=1}^{N}\sum_{t=1}^{\infty}\frac{Z_s Z_t}{r_{st}}$$

where e is the charge on the electron, N is the number of atoms in the unit cell, Z is the ionic charge of the atoms in the unit cell, and r_{st} is the distance between the sth and tth atoms.

A procedure with more rapid convergence was described by Bertaut (*5*) and used by Baur (*6*) to locate hydrogen atom positions in hydrated salt structures. The computations reported here were made with a modified version of Baur's computer program.

The orientation of the hydroxyl group in muscovite has been discussed by several authors on the basis of infrared absorption data from single crystals. Serratosa and Bradley (*7*) suggested that the O–H bond makes an angle of 15° to 20° with the cleavage plane and is directed toward the unoccupied octahedral site. Tsuboi (*8*) and Sutherland (*9*) favored an orientation pointing away from the octahedral layer. The most reliable study is that of Vedder and McDonald (*10*), who give an orientation of the O–H transition moment as making angles of 16° and 30° with the cleavage plane and the *b*-axis, respectively, in the *a*-*b* plane. They are very careful to point out that the actual OH bond need not coincide with the transition moment. The question of whether the bond points away from or toward the octahedral layer is not answered as clearly as one would wish (*11*). Their data suggest an orientation away from the octahedral layer.

I made my initial electrostatic energy calculations, using the atomic positional parameters of Radoslovich (*12*), the full ionic charge for each ion, and an assumed O–H distance of 0.97 Å. The OH vector was rotated about an axis approximately perpendicular to the cleavage plane, and the hydrogen ion positional parameters were calculated every 30° with reference to an arbitrary but constant origin. The angle between the rotation axis and the OH vector was varied in increments of 20°. In this manner a sampling of all possible hydrogen positional parameters was made and the electrostatic energy was calculated for each. The minimum value was determined by interpolation of these data points. The positional parameters (in fractions of the cell edge) for the hydrogen ion for the minimum energy are $x = 0.337$, $y = 0.640$, and $z = 0.059$. The OH bond makes angles of 8° and 40.5° with the cleavage plane and the *b*-axis, respectively, in the *a*-*b* plane and it points away from the octahedral layer. This orientation is approximately 11° away from the orien-

Table 1. Selected interatomic distances and angles for muscovite and muscovite without potassium (*18*).

Atom	Interatomic distance (Å)
Muscovite (Al–OH–H angles, 117° and 119°)	
H–O_a	2.94
O_a	2.80
O_a	2.72
O_b	2.94
O_b	2.85
O_b	2.69
Al	2.53
Al	2.53
K	3.74
Muscovite without K (Al–OH–H angles, 128° and 129°)	
H–O_a	3.06
O_a	2.84
O_b	2.88
O_c	2.94
O_d	2.40
O_e	2.89
Al	2.64
Al	2.63
(K)	3.23

tation of the transition moment as determined by Vedder and McDonald (*10*).

Gatineau (*13*) and Burnham and Radoslovich (*14*) have reported more accurate refinements of the muscovite structure. The structure described by Gatineau is derived from a least-squares refinement in which Radoslovich's x-ray intensities (*12*) were used. The Burnham and Radoslovich structure contains appreciable amounts of sodium and for this reason was not considered. The same procedure, as described earlier, was used to locate the minimum in electrostatic energy with Gatineau's positional parameters. The hydrogen positional parameters are $x = 0.371$, $y = 0.649$, and $z = 0.065$. The OH bond makes angles of 18° with the cleavage plane and 31° with the *b*-axis in the *a-b* plane and is 2.5° away from the transition moment orientation. Vedder (*15*) has suggested that the difference in orientation between the OH bond and the transition moment should not be more than 3°, an indication that the electrostatic energy approach described here is capable of considerable accuracy. In addition, the difference in the results obtained by use of the Radoslovich structure as opposed to the more accurate Gatineau structure indicates that the minimum in the electrostatic energy is very sensitive to errors in the atomic positional parameters.

Radoslovich (*16*) has suggested that, if the potassium ion were not present in the muscovite structure, the OH bond would make an angle of 60° to 70° with the cleavage plane. This result has been questioned by Farmer and Russell (*17*). For this reason I repeated the calculation of the electrostatic energy as described above (using the Gatineau structure) except that the potassium ion was excluded. The minimum value occurs when the OH bond makes angles of 53° and 30.5°, respectively, with the cleavage plane and the *b*-axis in the *a-b* plane. The positional parameters for the hydrogen are $x = 0.413$, $y = 0.617$, and $z = 0.089$. This result indicates how great is the influence of the interlayer cation on the hydroxyl orientation. Some selected interatomic distances and angles are listed in Table 1 for the hydrogen ion position in normal muscovite and in muscovite without potassium (*18*).

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18. The notation is that used by Radoslovich (*12*) in which the capital letters indicate the nature of the atom (OH = hydroxyl oxygen) and the subscripts distinguish atoms of the same kind that are not related by symmetry. The appearance of the same atom in the list more than once indicates interatomic distances to two or more atoms related by the space group symmetry.
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Polywater or Sodium Acetate?

Abstract. *Measurements of the infrared spectrum of sodium acetate suggest that high concentrations of this impurity may account for the unique spectrum of anomalous water.*

It has been suggested that the infrared spectrum of anomalous water (*1*) is unique and does not correspond to the spectrum of any known substance (*2*). This conclusion does not appear to be correct since the infrared spectrum of sodium acetate is remarkably similar to that of anomalous water. Electron microprobe examinations (*3*) have indicated the presence of large quantities of sodium impurity in the anomalous water, and Rabideau and Florin (*4*) have reproduced the physical properties ascribed to anomalous water with concentrated salt solutions such as sodium metaborate and sodium tetraborate decahydrate. However, although parts of the infrared

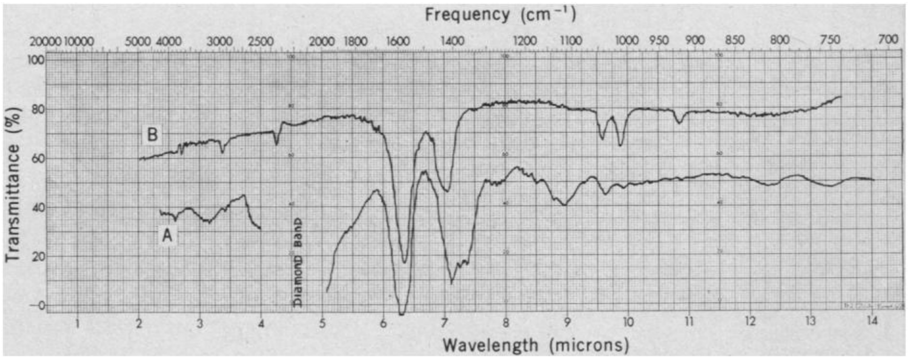

Fig. 1. Infrared spectrum of anomalous water on a diamond platelet (curve A) [reproduced from (*2*)]; infrared spectrum of sodium acetate on a silicon platelet (curve B). The spectrum of sodium acetate was recorded on a standard double-beam spectrometer (Perkin-Elmer model 21). The sample was deposited on the platelet from a methanol solution. The silicon platelet background (not shown) is flat.