

WISHERD and BONHAM⁴ of solid inorganic compounds shows that a mass relationship must also be operative in related series. For example the sulfate, phosphate, arsenate and tungstate of calcium have major bands which center (at half height) at 8.8, 9.4, 11.9 and 12.3 microns respectively. If these bands are correctly attributed to the stretching frequencies of the S—O, P—O, As—O and W—O pairs of the "anions", a reasonable linear relationship exists between the square of the wavelength and the respective reduced mass. The same is observed for the chlorate, bromate and iodate of sodium and for other series.

Returning to the quartz structures, it is evident that this relation very nearly holds for the GeO₂ and SiO₂ pair, and if the cation and anion charges are considered, also for BeF₂. The agreement is improved by introducing an empirical term for the electron content of the bonds involved⁵.

4. The most generalized case, of course, involves the interaction between coordination (CN), valence ($Z_A \cdot Z_X$), a reduced mass term (μ), the sum of atomic numbers ($A_A + A_X$)^{1/2}, and the absorption wave length. By purely empirical means the following relation was found to hold well for the simple AX₂ compounds (BeF₂, SiO₂, GeO₂) and the GeO₂ rutile form.

$$"K" = \frac{(CN)(\mu) \cdot (A_A + A_X)^{1/2}}{Z_A Z_X \cdot \lambda^2} = 0.168.$$

The agreement for these compounds is within ± 0.002 , or within 2 per cent.

Proceeding from the very restricted selection of AX₂ structures, to the more general ABO₄ compounds of the silica and rutile structures, the agreement does not hold as well, as a study of the figures of Table 1 will show. The "constant" calculated differs from 0.168 by 7.5 per cent on the average for this group, with individual values disagreeing as much as ± 17 per cent. That there exists some agreement even within these limits is of interest in view of the complications introduced by the change from simple binary compounds to ternary ones and the resulting possibilities of ordered and disordered arrangements.

⁴ J. M. HUNT, M. P. WISHERD and L. C. BONHAM, Infra-red absorption spectra of minerals and other inorganic compounds. Anal. Chem. **22** (1950) 1478-1497.

⁵ This electronic effect was found to be proportional to the 1/3 power of the sum of the metal-anion atomic numbers, that is, of the sum of extranuclear electrons. This factor probably can be rationalized as being proportional to the linear electronic density parallel to the stretching directions modifying the vibrations of the mass centers.

The use of

Table 1. Application

Compound	Form
BeF ₂	qtz.
SiO ₂	qtz.
GeO ₂	qtz.
GeO ₂	rutile
BPO ₄	qtz.
BAsO ₄	qtz.
AlPO ₄	qtz.
AlAsO ₃	qtz.
GaPO ₄	qtz.
GaAsO ₄	qtz.
FePO ₄	qtz.
GaSbO ₄	rutile

For the ABO₄ compounds the atomic number component is calculated as

In Table 2 there are AX₂ and ABX₄ compounds. The values are from works^{6,7,8}, and from data for this purpose here is to show that the values for different known forms of the glass, 3.6 per cent above, and quartz. The total per

⁶ Data on Chemicals, National Research Council, Washington, D. C.

⁷ J. D. H. DONNAY, Ann. Chim. Phys. **25** (1954) 1-10.

⁸ Standard X-Ray Diffraction Standards, Washington, D. C.