CALCULATION OF DENSITY FROM *X*-RAY DATA*

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In calculating densities of crystals from *x*-ray measurements it is necessary to understand clearly the reasons for differences in the values adopted for Avogadro's number, as noted by Pabst.[1] Pabst's warning should be strongly emphasized. Recent work in the Geological Survey on weinschenkite,[2] including a comparison of observed with calculated densities, has suggested the desirability of a more detailed examination of the factors involved in such calculations. Using the older value 6.060×10^{23} for Avogadro's number, Milton, Murata, and Knechtel calculate from *x*-ray measurements given by Strunz the density 3.270 for Virginia weinschenkite, in good agreement with their observed density 3.263. If they had erroneously used the newer absolute value 6.023×10^{23} for Avogadro's number, their calculated density would be 3.289, in poorer agreement with the observed value.

The present confusion with regard to the scales of *x*-ray wavelength was anticipated by Warren[3] in 1941, and has recently been discussed by Lipson and Riley,[4] Siegbahn,[5] and Wilson,[6] with tentative proposals for an unambiguous notation. Crystal cell dimensions are measured in terms of *x*-ray wavelengths by use of the well known Bragg equation

$$n\lambda = 2d \sin \theta.$$

The direct proportionality of the relation between the value for the wavelength λ of the *x*-rays and the value of the crystal dimension d shows the directly proportional effect of an error in the value of either quantity upon the other. Although the cell dimensions are usually measured on the Siegbahn scale of *x*-ray wavelengths, the reported values have been labeled "Ångstrom units" by most workers. The unit of the Siegbahn scale is not the Ångstrom unit, but the "*X*-unit," defined by an arbitrarily chosen value, 3029.04 X.U. at 18°,[7] for the interplanar distance of calcite crystals. This definition was arrived at by calculating the interplanar distance from the known values for the density and the molecular weight of calcite and for Avogadro's number;

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[1] Pabst, A., *Am. Mineral.*, **28,** 373 (1943).

[2] Milton, C., Murata, K. J., and Knechtel, M. M., *Am. Mineral.*, **29,** 92–107 (1944).

[3] Warren, B. E., *Jour. Applied Physics*, **12,** 383 (1941).

[4] Lipson, H., and Riley, D. P., *Nature*, **151,** 250, 502 (1943).

[5] Siegbahn, M., *Nature*, **151,** 502 (1943).

[6] Wilson, A. J. C., *Nature*, **151,** 562 (1943).

the value of Avogadro's number was the least accurately known of these quantities. Because Siegbahn chose the best values available at the time for these quantities, the *X*-unit is very nearly equal to one thousandth of an Ångstrom unit; but more recent experimental work has shown that the value of Avogadro's number is lower than the value $(6.0594 \pm 0.0063) \times 10^{23}$ assumed by Siegbahn.[7] This has been confirmed independently by two kinds of experiments. The success of experiments to measure the absolute wavelength of *x*-rays by diffraction from ruled optical gratings first showed a discrepancy between the absolute wavelength scale and the relative wavelength scale based on Siegbahn's assumed interplanar distance for calcite. Careful examination of the experimental results on which the Siegbahn scale was based threw suspicion on the formerly accepted value for the charge on the electron, from which Avogadro's number had been calculated, and when this value was redetermined the result agreed with the grating experiments.[8] As a result of this slight discrepancy, shifting the decimal by three places in the Siegbahn scale readings does not exactly give $10^5 \times$lengths expressed in centimeters, as does the "grating wavelength scale." However, when lattice volumes in Siegbahn units cubed are multiplied by the value for N contained in Siegbahn's "crystal wavelength scale," the incorrect value is cancelled out, so this is the proper value of N to use with lattice constants which are measured on the Siegbahn scale.

If for any reason the length of a lattice parameter in absolute Ångstrom units is wanted, it is found by multiplying the "Siegbahn" distance by the conversion factor $(\lambda_{\text{grating}}/\lambda_{\text{siegbahn}}) = 1.002034 \pm 0.000060$; similarly, volumes in Siegbahn units cubed must be multiplied by the cube of this conversion factor $(\lambda_g/\lambda_s)^3 = 1.0061 \pm 0.0002$, to get the volumes in absolute units. The "best" value of N is at present considered to be $(6.0228_3 \pm 0.0011) \times 10^{23}$ molecules per mole, where the molecular weight is expressed in "chemical atomic mass units." These values are based mainly on the work of Bearden.[9] Reported measurements should be carefully examined to see on which wavelength scale they are expressed.

In calculating the density of a crystal, $\rho = nM/Nv$, the product Nv should be the same whether got by multiplying the volume v of a unit cell in absolute cubic Ångstrom units by the correct value of N, or (since v is equal to the volume in Siegbahn units cubed multiplied by the cube of the wavelength scale conversion factor) by multiplying the volume in

[7] Siegbahn, M., *Spektroskopie der Röntgenstrahlen*, p. 43 (2nd ed., Berlin, 1931).

[8] An excellent critical and detailed summary of this work may be found in Stranathan, J. D., The "Particles" of Modern Physics, Philadelphia (1942).

Siegbahn units by $N(\lambda_g/\lambda_s)^3$. Using the "best" values given by Birge,[9] $N(\lambda_g/\lambda_s)^3 = (6.0597 \pm 0.0016) \times 10^{23}$, the proper value to use instead of N in calculations with cell volumes measured on the Siegbahn scale. This is practically identical with the value of N assumed by Siegbahn.[7]

The values given above are those for a mole of substance in "chemical atomic mass units," the scale on which atomic weights are reported by chemists. This scale is based on the arbitrarily assumed atomic weight of exactly 16 for the mixture of oxygen isotopes naturally occurring in air. In using data reported by physicists, care must be taken to note that another scale is often used, that of "physical atomic mass units," on which the pure oxygen isotope O^{16} is assigned the atomic weight of exactly 16. The conversion factors

1 physical atomic mass unit $= 0.999728 \pm 0.000005$ chemical atomic mass unit
1 chemical atomic mass unit $= 1.000272 \pm 0.000005$ physical atomic mass unit

are found from mass-spectrographic measurements of the relative abundance of the three oxygen isotopes O^{16}, O^{17} and O^{18} in air, by several workers (Birge[9]).

For convenience, the values to be used under the different circumstances mentioned are summarized in the accompanying table.

Molecular Weight in	Cell Dimensions Measured on	N, molecules per mole	1/N, grams per atomic mass unit
Chemical Atomic Mass Units	Siegbahn Scale	$(6.0597 \pm 0.0016) \times 10^{23}$	$(1.65026 \pm 0.00042) \times 10^{-24}$
	Grating Scale	$(6.0228 \pm 0.0011) \times 10^{23}$	$(1.66035 \pm 0.00030) \times 10^{-24}$
Physical Atomic Mass Units	Siegbahn Scale	$(6.0613 \pm 0.0016) \times 10^{23}$	$(1.64981 \pm 0.00042) \times 10^{-24}$
	Grating Scale	$(6.0245 \pm 0.0011) \times 10^{23}$	$(1.65990 \pm 0.00030) \times 10^{-24}$

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[9] Bearden, J. A., *Jour. Applied Physics*, **12**, 395–403 (1941).
Birge, R. T., *Reports on Progress in Physics*, **8**, 90–134 (1941). (London, *The Physical Society*, **1942**); *Rev. Mod. Phys.*, **13**, 233–239 (Oct. 1941).