Table 1. Strontium content, oxygen concentration, chlorinity, and temperature of Sargasso Sea water at station HS-195, 13 November 1963.

Depth (m)	O_2 (ml/liter)	Temp. (°C)	Cl (per mill)	Sr (mg-atom/liter)	Strontium-chlorinity ratio
25	4.96	22.80	20.175	0.097	0.00481
75	5.06	21.14	20.265	.096	.00474
100	4.79	19.96	20.242	.098	.00484
250	5.00	18.21	20.237	.098	.00484
500	4.63	—	20.106	.104	.00517
600	4.18	15.33	19.930	.118	.00592
800	3.45	11.08	19.586	.106	.00541
1000	4.40	6.69	19.405	.098	.00505
1400	5.93	4.32	19.359	.100	.00517
2595	6.05	3.12	19.339	.102	.00527

ratio 0.0048 if strontium is measured in milligram-atoms per liter and chlorine is measured in per millage.

In order to investigate seasonal and annual variations in physical, chemical, and biological properties of the Sargasso Sea, a standard oceanographic station (Station S), located 23 km southeast of Bermuda at 32°10′N, 64°30′ W, has been occupied by the Bermuda Biological Station research vessel *Panulirus* at intervals of approximately 2 weeks since 1954. The ocean depth is 3400 m. Water samples for strontium analyses were collected there from various depths (Table 1) during November 1963 with Nansen reversing bottles; temperatures were recorded with reversing thermometers mounted on the bottles. Soon after collection, the samples were analyzed for oxygen by the Winkler method and for salinity with an inductive salinometer (*2*). Polyethylene bottles were used to store the samples for strontium determinations—also made soon after collection. Immediately after collection and before analysis for strontium, the samples were filtered through a 0.45-μ Millipore filter to remove plankton and particulate matter. Strontium concentrations were determined by the flame photometric internal standards technique of Chow and Thompson (*1, 3*); the determinations are accurate within 0.002 mg-atom/liter. Resultant data are presented in Table 1 and Fig. 1.

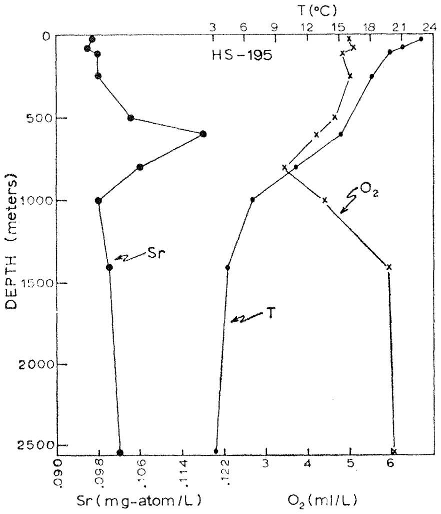

Fig. 1. Vertical distribution of strontium, oxygen, and temperature in Sargasso Sea water on 13 November 1963. Of special interest is the strontium concentration at 500 to 800 m.

The vertical distribution of strontium in waters below this station shows that the strontium-chlorinity ratio is variable (Table 1) and that there is a significant increase in strontium at 500 to 800 m (Fig. 1). Strontium-chlorinity ratios are correspondingly high at these depths (Table 1). The high strontium content is found at the permanent thermocline and lies near the top of the oxygen minimum zone. Chow and Thompson (*1*) reported a low strontium-chlorinity ratio for the oxygen minimum zone at 1000 m in the Pacific. They did not compute strontium-chlorinity ratios, but the data of Sugawara and Kawasaki (*4*) from the Western Pacific, Indian, and Antarctic oceans, recalculated by me, also indicate that the strontium-chlorinity ratios of those waters are variable.

Maxima at intermediate ocean depths have been reported for other trace elements. Recently cesium was found to be concentrated at 500 to 1500 m (*5*). It was suggested that the downward transport of cesium by particulate matter accounted for high concentrations at these depths.

The reasons for these relatively high strontium concentrations in Sargasso Sea water are still unknown, and only further investigation will show whether there are seasonal or other variations which can be correlated with oceanic processes. Solution of calcareous skeletons of organisms may occur at 500 to 800 m, releasing strontium; this could account for the relatively high strontium concentrations at these depths. However, it may be significant that the greatest concentration of organic aggregates is frequently found at 500 to 800 m (*6*); this is thought to arise through physico-chemical processes whereby dissolved organic materials in the water column are converted to particulate form on the surfaces of rising and bursting bubbles (*7*). Chemical bonding occurs during the conversion process, and some of the products may be insoluble organic compounds containing strontium. Reaction of these organic aggregates with the water may account for the higher strontium content and strontium-chlorinity ratio of these waters.

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20 July 1964

Crystal Structure of Weddellite

Abstract. *On the basis of x-ray analysis of its crystal structure, weddellite (the tetragonal crystal of calcium oxalate polyhydrate) has been determined to be a zeolitic dihydrate salt. The oxalate ion has at least the symmetry* 2mm *and possibly the symmetry* mmm. *The calcium ion is coordinated with eight oxygen atoms arranged in the form of a distorted cubic antiprism.*

The tetragonal form of crystals of hydrated calcium oxalate in certain plants and animals has been given the common name, weddellite (*1*). The hydrate stage of weddellite has been variously reported during the last 30 years. Frey-Wyssling (*2*), Klasens, Perdok, and Terpstra (*3*), and Pobeguin (*4*) found a formula weight of three molecules of water per molecule of salt. However, Honegger's measurements (*5*) indicate 2.5 molecules of water as the hydrate composition, while Bannister and Hey (*1*) and Gasser, Brauner, and Preisinger (*6*) reported that the tetragonal crystal of calcium oxalate is a dihydrate. Philipsborn (*7*) determined that weddellite is a dihydrate which can take up a maximum of one-half mole of zeolitic water per mole of salt. Most recently, Walter-Lévy and Laniepce (*8*) measured values of 2.27 to 2.32 for the ratio H_2O:Ca and accepted the figure 2.25 for the hydrate composition.

A presumptive specimen of weddellite, in the form of a kidney calculus of macroscopically individualized tetragonal crystals, was subjected to x-ray analysis. The x-ray diffraction diagram of the ground crystal powder was that of typical weddellite (*5*). Intensity data (720 independent reflections) were obtained with CuKα radiation from a single crystal, 0.25 by 0.1 mm, by photographic methods with the Weissnberg technique, the crystal being rotated about the [100] axis.

The space group is I4/m. (The structure could not be refined in the space groups I$\bar{4}$ and I4). The unit cell has the dimensions, $a = 12.30 \pm 0.02$ Å, $c = 7.34 \pm 0.02$ Å. Density by flotation is 2.00 g/ml, so that $Z = 8$.

The positions of the salt atoms and of the two water-oxygen atoms of a dihydrate were derived from the three-dimensional Patterson function. With these atoms, refinement of all the data by least squares reduced

$$R = \Sigma \, || F_{obs} | - | F_{calc} || \, / \, \Sigma \, | F_{obs} |$$

to 0.179. At this stage, three-dimensional Fourier synthesis of F_{obs}-$F_{calc.}$ and also F_{obs} alone showed an unaccounted-for peak density of about 2 to 3 electrons per cubic angstrom on the 4-fold axis, occupying the center of the only relatively open position within the unit cell. This peak was taken to represent the presence of a disordered water molecule at that site (a water molecule here would give the maximum hydrate condition of the salt as 2.5 H_2O). Placement of an oxygen atom in the indicated position improved *R* to 0.174, but the atom had an unusually large thermal parameter (17 Å^2). It appeared either that the atom was incorrectly placed (that the water molecule does not lie exactly on the 4-fold axis) or that—if the cell is zeolitic—there was not the equivalent of a full water molecule in this position. The first alternative was ruled out by calculation. On the basis of the second alternative, with 0.4 of an oxygen atom on the 4-fold axis (that is, corresponding to the formula $CaC_2O_4 \cdot 2.2\ H_2O$), *R* was lowered to 0.171, and the thermal parameter of the water oxygen was reduced to a more reasonable 5.7 Å^2. When a smaller fraction (0.2) of an atom was used, the thermal parameter became negative. The crystallographically determined water composition of this particular weddellite crystal thus is in accord with the measured density, which gives 2.17 H_2O per CaC_2O_4 moiety. Further least squares refinement, on the basis of assigning the unobserved intensities one-half the value of the smallest observed intensity, rather than zero, lowered *R* to 0.141. Treatment of the calcium ion as having anisotropic thermal movement gave only a slight improvement, with a final *R* value of 0.138. Without the unobserved intensities, *R* is 0.130.

Table 1. Atomic coordinates and thermal parameters in weddellite ($CaC_2O_4 \cdot 2.2\ H_2O$).

Atom	*x*	*y*	*z*	*B*, Å^2
Ca	0.200	0.300	0	(0.4)*
O (1)	.356	.246	0.181	1.0
O (2)	.537	.236	.180	2.2
O (w1)	.144	.114		1.8
O (w2)	.020	.386		2.6
O (w3)			.291	5.7
C	.445	.242	.105	0.9

* Isotropic *B* equivalent to average of anisotropic temperature factor.

Atomic coordinates and thermal parameters are given in Table 1. The calcium atom is coordinated with eight oxygen atoms (two water-oxygen atoms and six oxalate-oxygen atoms), which are roughly arranged in the form of a cubic anti-prism, with an average C–O distance of 2.45 Å. The oxalate ion is planar, and the C–C bond is bisected by a symmetry plane. Therefore the oxalate ion has at least the symmetry *2mm*, the bond lengths being C(1)–C(2), 1.55 ± 0.02 Å; C(1)–O(1), 1.23 ± 0.01 Å; C(1)–O(2), 1.26 ± 0.01 Å. The bond angles are C(2)–C(1)–O(1), 117.0 ± 0.5°, C(2)–C(1)–O(2), 115.9 ± 0.5°; O(1)–C(1)–O(3), 127.1 ± 0.8°. Because the differences between corresponding bond lengths and bond angles do not have statistical significance, it is conceivable that the symmetry of the oxalate ion here may be *mmm*.

Hydrogen atoms are not detectable with these data. Hydrogen bonds are assigned on the basis of appropriate lengths and angles to those O–O distances which appear to interconnect primitive cells: 2 [O(w1)–O(1)′], O(w2)–O(2)′, O(w2)–O(w2)′, with the respective bond distances, 2.91 ± 0.01 Å, 2.87 ± 0.01 Å, 2.84 ± 0.02 Å. The water molecule O(w3) is 3.06 ± 0.12 Å from the water oxygen O(w3)′, 3.11 ± 0.04 Å from the water oxygen O(w1), and 3.29 ± 0.01 Å from the oxalate oxygen O(2)′.

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High-Pressure Polymorphs in the Silver Iodide Phase Diagram

Abstract. *A good x-ray diffraction pattern has been obtained for the new phase of silver iodide stable in the vicinity of 3 kilobars at room temperature. A stability diagram of the six phases of silver iodide is presented to show the probable position of the narrow stability field of this phase. The x-ray diffraction data indicate that the cell symmetry of the new phase is probably orthorhombic.*

It now appears that silver iodide can exist in at least six polymorphic modifications. At room temperature and atmospheric pressure, that the stable form is hexagonal wurtzite type (II, Fig. 1) is evident from the careful work of