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RECENT PUBLISHED RESEARCH OF THE
KUYBYSHEV ENGINEERING INSTITUTE, MOSCOW

Standard Entropy of Metasilicates of Strontium, Barium, Zinc, Cadmium, Lead, and Iron," V. A. Kireev, Kuybyshev Eng Inst, Moscow

"Zhur Obshch Khimii" Vol 16, 1946, pp 1391-2

The calculation was made on the basis of Kelley's data for $S_{298.1}$ of $MgCO_3$, $ZnCO_3$, $PbCO_3$, $MnCO_3$, $FeCO_3$, $CaCO_3$ (calcite and aragonite), $SrCO_3$ (strontianite), and $BaCO_3$ (witherite) assuming for the entropy of formation, ΔS_f^s, from monatomic ideal-gaseous elements: $FeSiO_3$ 1.6 times that of $FeCO_3$, in analogy with $MnSiO_3$ and $MnCO_3$ (error not over ± 0.5); for $SrSiO_3$, $BaSiO_3$, $BaSiO_3$, $ZnSiO_3$, $CdSiO_3$, ΔS_f^s 1.9 times that of the carbonates (from $MgSiO_3$ and $MgCO_3$); for $PbSiO_3$, 1.7 times. This gives for ΔS_f^s: $MgSiO_3$ -174.9, $CaSiO_3$ -171.1, $SrSiO_3$ -171.2, $BaSiO_3$ -169.0, $ZnSiO_3$ -173.8, $CdSiO_3$ -170.0, $PbSiO_3$ -165.5, $MnSiO_3$ -175.8, $FeSiO_3$ -175.[illegible] cal/mole/degree. Hence, $S_{298.1}$ and ΔS_f^s from the elements in the standard state are: $FeSiO_3$ 23.0 ± 0.5, -61.5; $SrSiO_3$ 23.9 ± 2.0, -67.1; $BaSiO_3$ 27.2 ± 2.0, -67.0; $ZnSiO_3$ 29.2 ± 2.0, -67.8; $CdSiO_3$ 25.6 ± 2.0, -64.7; $PbSiO_3$ 32.0 ± 2.0, -61.6 cal/mole/degree, assuming for Sr(s) and Ba(s), S_{298} = 12.5 and 16.2, respectively. With the 18° values of the heats of formation, the approximate standard free energies of formation of $ZnSiO_3$ and $FeSiO_3$ are ΔF_f = -262.4 and -255.[illegible] kcal/mole, respectively.

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"A Method for Comparative Calculation of the Entropy, Heat, and Free Energy of Formation of Chemical Compounds: I. The Entropy of Formation of Inorganic Compounds From Atoms Under Standard Conditions," V. Kireev, Kuybyshev Inst Bldg Eng, Dept Chem, Moscow

"Acta Physicochimica USSR" Vol 20, 1945, pp 905-22

The attempt is made to establish some relations of a more general nature than the customary entropy of formation from simple substances. The concepts of atomic entropy of formation from free atoms, designated as ΔS_f^a, and the ideal entropy of formation from elements in a hypothetical state of a monatomic ideal gas at the same temperature and pressure p= 1 atmosphere, designated as ΔS_f^g, are introduced. The method is valuable for the heat of formation and free energy of formation also. The possibility of calculations is limited mainly by the incompleteness of data characterizing transition of various compounds to the ideal gas state, i.e., data on heat of vaporization, heat of sublimation, and saturated vapor pressure. The principal factor determining ΔS_f^a proves to be the number of atoms in a molecule of a given compound. Structural effects and position in Mendeleyev's periodic table modify the values of ΔS_f^a. The following generalization holds: transition within a single subgroup of the periodic table from elements with a lower atomic weight to heavier elements for similar compounds is accompanied by a gradual decrease of ΔS_f^a in absorption value. This applies to binary salts and oxides, but H is an exception to the rule. Mean values of ΔS_f^a are already sufficient to calculate the entropy of many compounds to within 1 to 5 EU per mole, according to the type of compound. Calculated values of ΔS_f^a are tabulated. In many cases the entropy values so calculated are sufficiently accurate for equilibrant calculations. Values of ΔS_f^a show that the function depends upon the number of atoms in the molecule to a greater extent than does ΔS_f^g for crystal substances. ΔS_f^a proves to be much more regular than the ordinary quantity ΔS_f. New calculations of entropy are given for NaBr, KI, $Ba(OH)_2$, HgI, $AgBrO_3$, $Mn(OH)_2$, $AgIO_3$, $KBrO_4$, $CsIO_4$, $Fe(OH)_2$, $CsBrO_4$, $Zn(OH)_2$, $CsMnO_4$, $Be(OH)_2$, $Sr(OH)_2$, and KIO_4. Entropy of CdO is calculated as 55.05 ± 0.5 instead of the published value of 46.9, and for TlI 69.9 instead of 63.9.

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