Calculated Thermodynamic Properties of Trimethylchlorosilane

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The vibrational assignment of trimethylchlorosilane has been revised, based on a normal coordinate treatment as a fourteen body problem[1]. The probable values of the wave numbers of the normal vibrations were used to calculate the values of the heat content, free energy, entropy and heat capacity for the ideal gaseous state at 1 atmospheric pressure (rigid rotator, harmonic oscillator approximation). The bond distances and the interbond angles in the previous Table I[1] and the Hirschfelder formula[2] were used to calculate the product of the principal moments of inertia, $I_aI_bI_b=3.85961\ 10^{-113}$ g^3 cm^6. The molecular weight used was 108.652 and the symmetry number was 3. The three torsional vibrational frequencies of the methyl groups belong to the species a_2 and e. No information about their frequencies has been given. Therefore, the total contributions of the translational, rotational and vibrational frequencies are listed in Table I, except those of the three unknown methyl torsional modes. When the contributions of the three ones are evaluated, they have to be added.

TABLE I. HEAT CAPACITY, FREE ENERGY AND HEAT CONTENT OF TRIMETHYLCHLOROSILANE FOR THE IDEAL GASEOUS STATE AT 1 ATMOSPHERIC PRESSURE (cal. deg^{-1} mol^{-1}), EXCEPT THE CONTRIBUTIONS OF THE THREE METHYL TORSIONAL FREQUENCIES

T°K	$(H^0-E_0^0)/T$	$-(F^0-E_0^0)T$	S^0	C_p^0
100	9.39	49.03	58.43	12.67
200	12.59	56.54	69.13	18.79
273.15	14.87	60.72	75.59	23.47
300	15.72	62.24	77.96	25.23
400	18.89	67.19	86.08	31.43
500	21.95	71.74	93.69	36.75
600	24.80	75.99	100.79	41.20
700	27.41	80.02	107.43	44.96
800	29.82	83.76	113.57	48.21
900	32.02	87.47	119.50	51.04
1000	34.05	91.01	125.05	53.51

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1) K. Shimizu and H. Murata, to be published in *J. Mol. Spectroscopy*.

2) J. O. Hirschfelder, *J. Chem. Phys.*, 8, 431 (1940).