

TABLE 1. *Typical entropy and free-energy contributions from translations, rotations, and vibrations at 298°K*

Motion		S° (cal deg <sup>-1</sup> mol <sup>-1</sup> )	H°-H <sub>0</sub> ° (kcal mol <sup>-1</sup> )	G°-H <sub>0</sub> ° (kcal mol <sup>-1</sup> )
Three degrees of translational freedom for molecular weights 20-200, standard state 1 M <sup>a</sup>		29-36	1.48	-7.2 to -9.1
Three degrees of rotational freedom <sup>a</sup>				
	Moments of inertia <sup>b</sup>			
Water	$5.8 \times 10^{-120}$	10.5 <sup>c</sup>	0.89	-2.24
<i>n</i> -Propane	$5.0 \times 10^{-116}$	21.5 <sup>c</sup>	0.89	-5.53
<i>endo</i> -Dicyclopentadiene	$3.8 \times 10^{-113}$	27.2 <sup>c</sup>	0.89	-7.21
Internal rotation <sup>d</sup>		3-5	0.3 <sup>e</sup>	-0.6 to -1.2
Vibrations <sup>a</sup>	$\omega$ , cm <sup>-1</sup>			
	1000	0.1	0.03	0.0
	800	0.2	0.05	-0.01
	400	1.0	0.20	-0.10
	200	2.2	0.35	-0.31
	100	3.4	0.46	-0.56

<sup>a</sup> Calculated from standard equations for translation (Sackur-Tetrode equation), rotation (rigid rotator), and vibration (assuming a harmonic oscillator) in the gas phase; see for example, Pitzer, K. S., and L. Brewer, *Thermodynamics* (McGraw-Hill Book Co., Inc., New York, 1961).

<sup>b</sup> Product of three principal moments of inertia, g<sup>3</sup> cm<sup>6</sup>.

<sup>c</sup> Symmetry corrected. <sup>d</sup> See text.

<sup>e</sup> Typical value; this quantity is a function of the barrier to rotation and the partition function.