

multiplied by the transmission coefficient, which is asymptotically  $\frac{1}{2}$  at the top of the barrier, so that Kramers' original formula is obtained. Alternately, the first boundary condition Eq. (3.4) could be changed to  $\sigma(x_1)=0$  and the first boundary condition for the expected

time could be changed to  $T(x_1)=0$ , where  $x_1 \gg x_0$ . If this is done, the asymptotic analysis of Eqs. (3.5) and (3.11) give Kramers' original result. We note that the agreement with transition state theory will be even worse, if these modifications are made.

## Erratum: Perturbation theory for the free energy of hard quadrupolar diatomics [J. Chem. Phys. 70, 5751 (1979)]

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In Eq. (2.12),  $-4g_{221}^{\text{HHD}}(r)$  should be  $+4g_{221}^{\text{HHD}}(r)$ . [In Eq. (23) of Ref. (10), the  $U_Q^{\text{PERT}}(r_{12})|_{221}$  should be of positive sign.] As emphasized in the text, the large differences between the results for the 500-particle Monte Carlo runs and the 256-particle runs demonstrate that the Monte Carlo data are insufficiently precise to yield reliable  $\Delta f_1$  estimates, although the order of magnitude of the estimates establish that the  $\Delta f_1$  contributions are small compared to the  $\Delta f^P$  contributions.

The  $y$  values for  $L=0.6$  shown in Tables III, V, and VI are displaced; they are entered correctly in the Table below. In Eq. (2.6),  $1/4$  should be  $y$ , while Eq. (2.7) should be

$$\beta \Delta f_0^B = \frac{(2\gamma - 3) + 2(\gamma^2/9 - \gamma + 3)y - 3y^2}{2(1-y)^2} - (1 - \gamma^2/9) \ln(1-y) + \ln y, \quad (2.7)$$

necessitating a change in the entries for Eq. (2.7) in Table III. The corrected entries, along with Fig. 1 redrawn in accordance with the corrected Table V is available from each author. We are grateful to W. A. Steele for pointing out a sign error in Eq. (2.12).

This changes the  $\beta \Delta f_1 Q^2$  entries of Table V, which should be as below:

		Corrections to TABLE V		
$\rho^*$	$y$	$\beta \Delta f_1 Q^2$		
		$L = 0.4$ ( $\text{N}_2$ )		
		$T = 20.7^b$ K	$T = 77.4$ K	$T = 126.1$ K
0.2		-0.0128	-0.0034	-0.0021
0.3		-0.0217	-0.0058	-0.0036
0.4		+0.0576	+0.0154	+0.0095
0.5 <sup>a</sup>		-0.0652	-0.0174	-0.0107
0.6		+0.0920	+0.0246	+0.0151
0.6 <sup>a</sup>		-0.0903	-0.0241	-0.0148
		$L = 0.6$ ( $\text{Cl}_2$ )		
		$T = 172$ K	$T = 238.6$ K	$T = 417$ K
0.2	0.1877	-0.0414	-0.0298	-0.0171
0.3	0.2815	-0.0409	-0.0295	-0.0169
0.4	0.3753	-0.0682	-0.0492	-0.0282
0.5	0.4692	-0.4006	-0.289	-0.165
0.6	0.5620	...	...	...

<sup>a</sup>500 particles.

<sup>b</sup>Although  $T = 20.7$  K is used as a reference  $T$  for the  $L = 0.4$  fluid in Ref. 10 and elsewhere, it is actually far too low a temperature to be relevant to the fluid state. (In  $\text{N}_2$ , the triple point is at 63.1 and an orientational-ordering transition takes place at  $\sim 35$  K.)