COMMENTS

Comment on "Molecular Properties of C_{60} in the Gas and Solid Phases" *J. Phys. Chem.* 1992, *96,* 858

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Received: January 19, 2003; In Final Form: April 16, 2003

Girifalco[1] proposed an analytic intermolecular potential for C_{60} in 1992. The expression is as follows:

$$\phi(r) = -\alpha\left[\frac{1}{s(s-1)^3} + \frac{1}{s(s+1)^3} - \frac{2}{s^4}\right] + \beta\left[\frac{1}{s(s-1)^9} + \frac{1}{s(s+1)^9} - \frac{2}{s^{10}}\right] \quad (1)$$

$s = r/2a$, r is the distance between two C_{60} centers, a is the radius of the C_{60} molecule and is equal to 0.355 nm. In Girifalco's paper, $\alpha = 74.94 \times 10^{-15}$ erg, and $\beta = 135.95 \times 10^{-18}$ erg. In 1994, Wales[2] used the intermolecular potential to study the rearrangement of $(C_{60})_{55}$ clusters.

In Girifalco's paper, the second virial coefficient $B(T)$ was calculated by using the equation

$$B(T) = -2\pi N_a \int_0^\infty [e^{-\phi(r)/kT} - 1] r^2 \, dr \quad (2)$$

k is Boltzmann's constant and N_a is Avogadro's number. In the integration of eq 2, the range of r is from 0 to ∞.

As we know, when $s \le 1$ (i.e., $r \le 2a$), two C_{60} molecules overlap, and $\phi(r)$ must be very large. But when $s \le 1$ (i.e., $r \le 2a$), in eq 1 $\phi(r)$ is not very large, so when $s \le 1$ (i.e., $r \le 2a$), Girifalco's interaction potential for two C_{60} molecules is not correct. When $s > 1$ (i.e., $r > 2a$), the potential describes the interaction between two C_{60} molecules well. Thus, Girifalco's analytical intermolecular potential for C_{60} could be modified as follows:

$$\phi(r) = \begin{cases} \infty & (s \le 0) \\ -\alpha\left[\frac{1}{s(s-1)^3} + \frac{1}{s(s+1)^3} - \frac{2}{s^4}\right] + \beta\left[\frac{1}{s(s-1)^9} + \frac{1}{s(s+1)^9} - \frac{2}{s^{10}}\right] & (s > 0) \end{cases} \quad (3)$$

Because eq 1 is incorrect for $s \le 1$, using eq 2 to calculate the second virial coefficient $B(T)$ could not give the correct values. When substituting eq 3 into eq 2 to calculate the second virial coefficient $B(T)$, the $B(T)$ equation could be rewritten as the following:

$$B(T) = -2\pi N_a \int_0^\infty [e^{-\phi(r)/kT} - 1] r^2 \, dr = 2\pi N_a \frac{8a^3}{3} - 2\pi N_a \times 8a^3 \int_1^\infty [e^{-\phi(s)/kT} - 1] s^2 \, ds \quad (4)$$

In the integration of eq 4, the range of r is from 1 to ∞.

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TABLE 1: Second Virial Coefficient $B(T)$[a] at Different Temperatures for C_{60}

temp, K	$-B(T)$, this paper	$-B(T)$, Girifalco[b]	temp, K	$-B(T)$, this paper	$-B(T)$, Girifalco[b]
490	168 246	57 530	700	30 453	13 160
500	149 757	51 990	725	26 616	11 730
510	133 955	47 210	750	23 476	10 530
520	120 373	43 030	775	20 876	9529
530	108 636	39 380	800	18 700	8674
540	98 445	36 160	850	15 292	7309
550	89 552	33 320	900	12 777	6276
560	81 758	30 800	950	10 865	5473
570	74 898	28 560	1000	9376	4835
580	68 834	26 550	1050	8192	4319
590	63 455	24 750	1100	7233	3894
600	58 665	23 130	1150	6443	3539
620	50 547	20 350	1200	5785	3239
640	43 982	18 050	1300	4753	2760
660	38 610	16 140	1400	3987	2400
680	34 166	14 530			

[a] The units of $B(T)$ are cm^3/mol. [b] See ref 1.

TABLE 2: Second Virial Coefficient $B(T)$[a] Recalculated by Girifalco and Independently by M. Hodak at Different Temperatures for C_{60}

temp, K	$-B(T)$	temp, K	$-B(T)$
450	286 500.76	950	11 076.38
500	151 281.06	1000	9578.96
550	90 442.04	1050	8388.25
600	59 257.51	1100	7424.01
650	41 603.24	1150	6630.65
700	30 802.20	1200	5968.76
750	23 772.39	1250	5409.71
800	18 961.85	1300	4932.36
850	15 531.40	1350	4520.79
900	12 999.67	1400	4162.84

[a] The units of $B(T)$ are cm^3/mol.

When substituting $a = 0.355$ nm into eq 4, $B(T)$ is given by

$$B(T) = 451.41 - 1354.24 \int_1^\infty [e^{-\phi(s)/kT} - 1] s^2 \, ds \ (cm^3/mol) \quad (5)$$

By using eq 5 and performing the integration numerically, the second virial coefficient $B(T)$ at different temperatures for C_{60} could be calculated. The results are listed in Table 1. For comparison, the $B(T)$ values of Girifalco for C_{60} are also listed in Table 1.

From Table 1, it can be seen that the $B(T)$ values from this paper are much larger than those of Girifalco's,[1] so the second virial coefficients in Girifalco's 1992 paper are not correct.

Recently, a recalculation of the second virial coefficients performed by Girifalco and independently by M. Hodak at North Carolina State University confirmed my results with some small differences.[3] The results of Girifalco and M. Hodak are listed in Table 2.

Comparing the results in Table 1 and those in Table 2, one can see that the differences are small and are due to differences in the accuracy of the numerical integration. Girifalco believes that his integration procedure is extremely accurate, and I agree with him.

Acknowledgment. This work was supported by the NSFC (20271043).

References and Notes

(1) Girifalco, L. A. *J. Phys. Chem.* **1992**, *96*, 858.
(2) Wales, D. J. *J. Chem. Phys.* **1994**, *101*, 3750.
(3) In the report of the reviewer.

10.1021/jp034150i CCC: $25.00
Published on Web 06/05/2003