(4) Cope, J.Q., Lewis, W.K., Weber, J.C., *Ibid.,* **23**, 887 (1931).
(5) Din, F., Ed., "Thermodynamic Functions of Gases," Vol. **3**, Butterworths, London, 1961.
(6) Dodge, B.F., *Ind. Eng. Chem.* **24**, 1353 (1932).
(7) Edmister, W.C., *Ibid.,* **30**, 352 (1938).
(8) Gamson, B.W., Watson, K.M., *Natl. Petrol. News, Tech. Sec.* **36R623** (Aug. 2 and Sept. 6, 1944).
(9) Gelles, E., Pitzer, K.S., *J. Am. Chem. Soc.* **75**, 5259 (1953).
(10) Hougen, O.A., Watson, K.M., "Chemical Process Principles," Part II, Wiley, New York, 1943.
(11) Hsu, C.C., McKetta, J.J., *A.I.Ch.E. J.* **9**, 794 (1963).
(12) Kordbachen, R., Tien, C., *Can. J. Chem. Eng.* **37**, 162 (1959).
(13) Lewis, W.K., Luke, C.D., *Trans. A. S. M. E.* **54**, 55 (1932).
(14) Lydersen, A.L., Greenkorn, R.A., Hougen, O.A., "Generalized Thermodynamic Properties of Pure Fluids," University of Wisconsin Engineering Experiment Station, Rept. 4 (1955).
(15) Nelson, L., Obert, E.F., *A.I.Ch.E. J.* **1**, 74 (1955).
(16) Newton, R.H., *Ind. Eng. Chem.* **27**, 302 (1935).
(17) Perry, J.H., Ed., "Chemical Engineers' Handbook," 4th ed., McGraw-Hill, New York, 1963.
(18) Pitzer, K.S., Lippmann, D.Z., Curl, R.F., Jr., Higgins, C.M., Petterson, D.E., *J. Am. Chem. Soc.* **77**, 3427, 3433 (1955); **79**, 2369 (1955).
(19) Reid, R.C., Sherwood, T.K., "Properties of Gases and Liquids," 2nd ed., McGraw-Hill, New York, 1966.
(20) Selheimer, C.W., Souders, Mott, Jr., Smith, R.L., Brown, G.G., *Ind. Eng. Chem.* **24**, 515 (1932).
(21) Seshadri, D.N., Viswanath, D.S., Kuloor, N.R., *J. Indian Inst. Sci.* **48**, 65 (1966).
(22) *Ibid.,* **49**, 117 (1967).
(23) *Ibid.,* **50**, 179 (1968).
(24) Silverberg, P.M., Wenzel, L.A., J. Chem. Eng. Data **10**, 363 (1965).
(25) Su, G.J., Sc.D. thesis, Massachusetts Institute of Technology, Cambridge, Mass., 1937.
(26) Tanner, H.G., Benning, A.F., Mathewson, W.F., *Ind. Eng. Chem.* **31**, 878 (1939).
(27) van der Waals, J.D., *Proc. Roy. Acad. Amsterdam* **132**, 315 (1908).
(28) Viswanath, D.S., "Thermodynamic Properties of Real Gases," Ph.D. thesis, University of Rochester, Rochester, N. Y., 1962.
(29) Viswanath, D.S., Su, G.J., *A.I.Ch.E. J.* **11**, 202 (1965).
(30) Watson, K.M., *Ind. Eng. Chem.* **35**, 398 (1943).
(31) Watson, K.M., Nelson, E.F., *Ibid.,* **25**, 880 (1933).
(32) Watson, K.M., Smith, R.L., *Natl. Petrol. News,* **28**, 29 (July 1936).

Transport Collision Integrals for Gases Using the Lennard-Jones (6, n) Potentials

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The three-parameter Lennard-Jones (6, n) intermolecular potential function was used to calculate the first six reduced collision integrals, the correction factors, and the various quantities derived from those collision integrals. The ranges of tabulation were

$n = 8(2)20$ and
$T^* = 0.001(0.005)0.02(0.01)0.1(0.05)0.5(0.1)1.0(0.2)$
$2.0(0.5)4.0(1.0)10(2.0)20(5)50(10)100$

[numbers in parentheses between two numbers were interval for tabulation]. The three intermolecular potential parameters—n, ϵ/k, and σ—were determined from the experimental viscosity data for 12 gases: helium, argon, neon, hydrogen, nitrogen, oxygen, carbon monoxide, carbon dioxide, air, methane, propane, and n-pentane.

THE TRANSPORT properties of a dilute gas can be calculated if the intermolecular potential energy function is known, and calculations of this kind have important applications in analyzing experimental data to provide information on the potential energy function and in interpolating or extrapolating experimental data. The calculation is based on the Chapman-Enskog solution of the Boltzmann equation, which is given by Hirschfelder, Curtiss, and Bird (9); it involves evaluation of collision integrals which are complicated integrals requiring three stages of numerical integration. These collision integrals have been tabulated for a number of potential energy functions, including the well known Lennard-Jones (6, 12) (9), Buckingham exp-6 (21), L-J (6, 9) (27), and L-J (7, 28) (27) functions. There is a large amount of evidence that these functions are not sufficiently flexible to describe the actual interactions of real molecules accurately. With the availability of high-speed computers, we have used the L-J (6, n) potentials to calculate collision integrals. Thus, the potential function allows the adjustable steepness of the repulsive potential an additional degree of flexibility as compared to the L-J (6, 12) potential. The applicability of the poten-

tials was tested for 12 gases with experimental viscosity data. Recently Klein and Smith (17) also tabulated collision integrals using L-J (6, n) with n = 9, 12, 15, 18, 21, 24, 30, 50, and 75.

The form of the L-J (6, n) potential $E(r)$ is

$$E(r) = \frac{n\epsilon}{n-6}\left(\frac{n}{6}\right)^{\frac{6}{n-6}}\left[\left(\frac{\sigma}{r}\right)^n - \left(\frac{\sigma}{r}\right)^6\right] \qquad (1)$$

where ϵ is the depth of the potential well, n is an adjustable parameter for the steepness of the repulsion potential, and $E(\sigma) = 0$. The reduced form of the potential is shown in Figure 1 for $n = 8$ and $n = 20$. This function should prove useful on several counts—it is simple in form, the repulsive index, n, serves as a simple indicator of the hardness of the repulsive core, the potential has been used in a number of more complicated theories (10, 23), this form has proved useful because the theory involves derivatives of potential which then leads to simple recursion formulas on the index n, and the potential functions derived
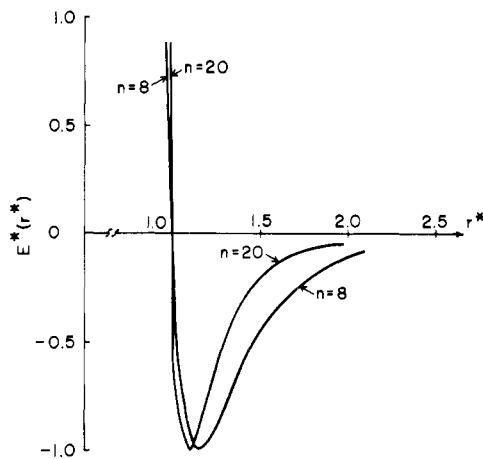
Figure 1. Reduced Lennard-Jones $(6, n)$ potential function for $n = 8$ and $n = 20$

from two-body scattering data have often been represented by simple inverse powers of the intermolecular distance $(1, 4, 23)$.

GENERAL FORMULAS

The transport properties (viscosity, thermal conductivity, diffusion coefficients, and thermal diffusion ratio) can all be calculated if the reduced collision integrals $\Omega^{l, s}{}^*$ are known. These integrals are defined by the equations (9):

$$\Omega^{l, s}{}^*(T^*) = \frac{1}{(s+1)! \, T^{*s+2}} \cdot \int_0^\infty e^{-g^{*2}/T^*} (g^{*2})^{s+1} Q^{l}{}^*(g^{*2}) d(g^{*2}) \tag{2}$$

$$Q^{l}{}^*(g^{*2}) = \frac{1}{\left[1 - \frac{1 + (-1)^l}{2(1+l)} \right]} \int_0^\infty (1 - \cos^l \chi) db^{*2} \tag{3}$$

$$\chi(g^{*2}, b^{*2}) = \pi - 2b^* \int_{r_m^*}^\infty \frac{dr^*/r^{*2}}{\left[1 - \left(\frac{b^*}{r^*}\right)^2 - \frac{E^*(r^*)}{g^{*2}} \right]^{1/2}} \tag{4}$$

The first approximations of various transport coefficients given in terms of collision integrals nowadays often appear elsewhere (9). Thus, there is no need to repeat these formulas. Higher approximations are obtained by multiplying the first approximation for the transport coefficients by correction factors which are near unity. Certain ratios of the collision integrals appear in the transport properties of mixtures (15). These ratios, being slowly varying functions of T^*, are also useful in interpolation. The ratios of collision integrals and the correction factors (15) are

$$A^* = \Omega^{2, 2}{}^*/\Omega^{1, 1}{}^* \tag{5}$$

$$B^* = [5\Omega^{1, 2}{}^* - 4\Omega^{1, 3}{}^*]/\Omega^{1, 1}{}^* \tag{6}$$

$$C^* = \Omega^{1, 2}{}^*/\Omega^{1, 1}{}^* \tag{7}$$

$$E^* = \Omega^{2, 3}{}^*/\Omega^{2, 2}{}^* \tag{8}$$

$$F^* = \Omega^{3, 3}{}^*/\Omega^{1, 1}{}^* \tag{9}$$

$$f_\eta = 1 + (3/196) (8E^* - 7)^2 \tag{10}$$

$$f_\lambda = 1 + (1/42) (8E^* - 7)^2 \tag{11}$$

$$f_D = 1 + (1/8) (6C^* - 5)^2 (2A^* + 5)^{-1} \tag{12}$$

where subscripts η, λ, and D are the viscosity, thermal conductivity, and self-diffusion coefficients, respectively.

NUMERICAL RESULTS

The numerical evaluation of the various integrals was carried out on an IBM 7040 computer. The calculation of the angle of deflection is complicated by the phenomenon of orbiting. The integrand of Equation 4 has a sharp maximum in the vicinity of the orbiting region. This difficulty may be alleviated by increasing the number of intervals of integration. Equation 4 was integrated numerically using the Gaussian 24-point quadrature formula with the interval of integration divided into two subintervals and then the Gaussian 32-point quadrature formula was used in each subinterval. Accuracy up to seven significant figures was attained for nonorbiting collisions and up to five significant figures for orbiting collisions.

The numerical calculation of the cross section becomes complicated when orbiting takes place in the encounter. To facilitate the calculation, Equation 3 may be rewritten in terms of r_m^* rather than b^{*2}, which gives

$$Q^{l}{}^*(g^{*2}) = A \int_{r_m^*}^\infty [1 - \cos^l \chi] H(g^{*2}, r_m^*) d(r_m^{*2}) \tag{13}$$

where

$$H(g^{*2}, r_m^*) = 1 - [E^*(r_m^*) + 0.5 \, r_m^* \, dE^*(r_m^*)/dr_m^*]/g^{*2} \tag{14}$$

$$A = 1 - \frac{1 + (-1)^l}{2(1+l)} \tag{15}$$

For nonorbiting collisions, the Gaussian 24-point quadrature formula was used to evaluate Equation 13 with the interval divided into two subintervals. Precision of six or seven figures was obtained. When orbiting collisions occur, the term $\cos^l \chi$ oscillates violently as the angle of deflection, χ, approaches negative infinity. The factor $H(g^{*2}, r_m^*)$ damps the oscillations as $H(g^{*2}, r_m^*)$ approaches zero at $r_m^* = r_n^*$. For the case of orbiting collisions, the interval of integration from r_{mo} to infinity is no longer continuous. Dividing Equation 13 into two parts at the point of discontinuity, one obtains

$$Q^{l}{}^*(g^{*2}) = A \int_{r_m^*}^{r_n^{*2}} [1 - \cos^l \chi] H(g^{*2}, r_m^*) d(r_m^{*2}) + A \int_{r_n^*}^\infty [1 - \cos^l \chi] H(g^{*2}, r_m^*) d(r_m^{*2}) \tag{16}$$

To evaluate Equation 16 efficiently, the interval of integration was divided into four regions:

Region 1 (from $\chi = \pi$ to $\chi = -2\pi$). The interval of integration from r_{mo}^{*2} (where $\chi = \pi$) to r_1^* (where $\chi = -2\pi$) was divided into two subintervals, using r_m^{*2} as an independent variable in the integration. Then the Gauss 32-point quadrature formula was applied in each subinterval.

Region 2 (from $\chi = -2\pi$ to $\chi = -\infty$). From r_1^{*2} to r_m^{*2} (where $\chi = -\infty$), the angle of deflection may be approximated by

$$\chi = \pi + C \ln |b_0^{*2} - b^{*2}| \tag{17}$$

where C is the constant to be determined. Then Equation 13 can be integrated analytically. If one defines

$$W_0 = |b_0^{*2} - b_1^{*2}| \tag{18}$$

and

$$W_k = |b_0^{*2} - b_1^{*2}| \, |kC_1 \sin (K\chi_1) + \cos (\chi_1)| / (1 + K^2 C_1^2) \tag{19}$$

in which χ_1 and b_1^{*2} are the values at $r_m^{*2} = r_1^{*2}$, the contributions to $Q^{l}{}^*(g^{*2})$ from this orbiting region are:

$$q^{1}{}^*(g^{*2}) = W_0 - W_1 \tag{20}$$

$$q^{2}{}^*(g^{*2}) = \frac{3}{4} (W_0 - W_2) \tag{21}$$

and

$$q^{3*}(g^{*2}) = W_0 - \tfrac{3}{4} W_1 - \tfrac{1}{4} W_3 \qquad (22)$$

The constant C was evaluated by a least-squares curve-fitting method. A total of 128 Gaussian points was used to evaluate the angle of deflection, χ.

Region 3 (from $\chi = -\infty$ to $\chi \doteq -2\pi$). The contributions to $Q^{l*}(g^{*2})$ from this orbiting region are found in exactly the same manner as in Region 3, except that C is evaluated from this side of the orbiting region.

Region 4 (from $\chi \doteq -2\pi$ to $\chi = 0$). The interval of integration from r_2^{*2} (where $\chi \doteq -2\pi$) to infinity (where $\chi = 0$) was divided into two subintervals, using $U = r_2^{*2}/r_m^{*2}$ as the new variable of integration. Then the Gauss 32-point quadrature formula was applied to each subinterval.

The over-all precision is estimated to be 0.05%. The largest contributions to the $Q^{l*}(g^{*2})$ come from Region 1. The contributions from other collision regions account for less than 1%.

The Fortran program for the computation of $Q^{l*}(g^{*2})$ contained a subprogram for calculating the angle of deflection. For each of seven values of the repulsion index n ($n = 8, 10, 12, 14, 16, 18, 20$), the $Q^{l*}(g^{*2})$ were calculated for $l = 1, 2, 3$ and for g^{*2} from 0.1 to 1000.

Equation 2 was used to calculate the reduced collision integrals by using the Laguerre 32-point quadrature formula (24) with $\exp(-g^{*2}/T^*)$ as the weight function. Only the first 16 points were required in the calculations, since the contributions to the collision integrals from the remaining 16 points were completely negligible. The values of Q^{l*} in Equation 2 were obtained by a four-point Lagrangian interpolation formula from the results tabulated from Equation 3. The Gauss quadrature formulas were used in the integration of Equations 3 and 4.

Table I gives the first six reduced collision integrals and Table II the higher approximation correction factors—f_η, f_λ, and f_D—and the various ratios of collision integrals. The collision integrals for the L-J (6, 12) potential obtained in this work are in good agreement with those calculated by Monchick and Mason (22), Itean, Gluck, and Svehla

(11), Barker, Fock, and Smith (2), and Klein and Smith (17). $\Omega^{1,1*}$ and $\Omega^{2,2*}$ for L-J (6, 12) are compared with Klein and Smith's work (17) in Table III (16). At reduced temperature below 0.6 both tables show internal differences indicating lower precision. In the neighborhood of 0.8 this work appears to be smoother than Klein and Smith's work, and between 0.8 and 2.0 Klein and Smith's appear to be smoother. In general, the agreement is excellent. Thus the accuracy of the calculation above $T^* = 0.1$ appears to be at least 0.1%. The uncertainty increases, with the reduced temperature becoming lower.

DETERMINATION OF POTENTIAL PARAMETERS

The intermolecular potential parameters were determined from experimental viscosity data by nonlinear least squares curve fitting to the formula for the viscosity of a pure gas given by Hirschfelder et al. (9).

$$\eta = \frac{5}{16} \left(\frac{MkT}{\pi} \right)^{1/2} \frac{f_\eta}{\sigma^2 \Omega^{2,2*}(T^*)} \qquad (23)$$

The technique is based on the Marquardt's (20) maximum neighborhood algorithm for the least-squares estimation of parameters in nonlinear formulas. The algorithm is a combination of the Taylor series method and the steepest descent (or gradient) method. In using Equation 23, two simplifications were made: The correction factor, f_η, was assumed to be unity, which is consistent with the experimental accuracy of the viscosity data, and the repulsive potential indices were confined to the values of 8, 10, 12, 14, 16, 18, and 20, at which the calculations were made.

The procedures used in the computer program for the determination of the potential parameters, n, ϵ/k, and σ were:

1. The repulsive potential index was first assumed to be 8; thus, the values of $\Omega^{2,2*}$ were found from Table I for the given repulsion index, $n = 8$. Then, an approximate value of σ and the experimental viscosity were stored in the computer along with the above information.

Table I. Collision Integrals for the
Lennard-Jones (6, n) Potentials

	$n = 8$		$n = 12$		$n = 20$	
T^*	$\Omega^{1,1*}$	$\Omega^{2,2*}$	$\Omega^{1,1*}$	$\Omega^{2,2*}$	$\Omega^{1,1*}$	$\Omega^{2,2*}$
0.010	9.2683	9.8176	6.6939	7.3970	5.5703	6.2542
0.050	6.4813	6.4475	4.9500	5.1317	4.1117	4.3539
0.100	5.1099	5.0693	3.9922	4.0957	3.3218	3.4866
0.500	2.3319	2.5953	2.0634	2.2898	1.8566	2.0282
1.000	1.5059	1.6882	1.4419	1.5913	1.3796	1.5085
5.000	0.7953	0.8932	0.8431	0.9267	0.8991	0.9631
10.000	0.6780	0.7723	0.7421	0.8243	0.8188	0.8822
50.000	0.4848	0.5629	0.5758	0.6496	0.6892	0.7486
100.000	0.4179	0.4900	0.5166	0.5849	0.6425	0.7006

Table III. Comparison of $\Omega^{1,1*}$ and $\Omega^{2,2*}$ of Lennard-Jones
(6, n) Potential with Klein and Smith's Values (17)

	$\Omega^{1,1*}$			$\Omega^{2,2*}$		
T^*	$\dfrac{[(KS) - (LH)]}{(KS)} \cdot 10^3$	K − S	L − H	$\dfrac{[(KS) - (LH)]}{(KS)} \cdot 10^3$	K − S	L − H
0.10	5.1240	4.0127	3.9922	1.9825	4.1039	4.0958
0.50	1.3720	2.0662	2.0634	1.3446	2.2867	2.2898
1.00	1.7968	1.4394	1.4420	1.2599	1.5933	1.5913
5.00	0.4756	0.8427	0.8431	0.0777	0.9266	0.9267
10.00	0.1496	0.7422	0.7421	0.1759	0.8242	0.8244
50.00	0.0521	0.5759	0.5759	0.0231	0.6496	0.6497
100.00	0.2303	0.5167	0.5166	0.2342	0.5851	0.5850

Table II. Higher Approximation Correction Factors for Lennard-Jones (6, n) Potentials

	$n = 8$			$n = 12$			$n = 20$		
T^*	f_η	f_λ	f_D	f_η	f_λ	f_D	f_η	f_λ	f_D
0.010	1.0071	1.0110	1.0099	1.0085	1.0133	1.0112	1.0086	1.0134	1.0111
0.050	1.0016	1.0025	1.0024	1.0021	1.0033	1.0033	1.0022	1.0034	1.0032
0.100	1.0013	1.0021	1.0012	1.0017	1.0027	1.0020	1.0018	1.0029	1.0021
0.500	1.0005	1.0008	1.0012	1.0000	1.0000	1.0000	1.0006	1.0009	1.0003
1.000	1.0006	1.0010	1.0004	1.0000	1.0000	1.0000	1.0003	1.0004	1.0007
5.000	1.0043	1.0067	1.0041	1.0058	1.0090	1.0059	1.0075	1.0117	1.0082
10.000	1.0056	1.0088	1.0056	1.0073	1.0114	1.0076	1.0092	1.0144	1.0101
50.000	1.0052	1.0081	1.0055	1.0075	1.0117	1.0081	1.0097	1.0152	1.0199
100.000	1.0055	1.0086	1.0058	1.0073	1.0114	1.0080	1.0100	1.0167	1.0113

Table IV. Potential Parameters Determined from Viscosity Data

Gas	n	η/k, °K.	σ, A.	Temperature Range, °K.	No. of Data Points Used	Standard[a] Error	Data Sources
He	10	10	2.650	80.0–1088.0	31	0.085	(13, 30)
Ar	14	130	3.390	80.0–1500.0	44	0.217	(6, 13, 31)
Ne	14	45	2.715	80.0–1000.0	14	0.170	(13)
H_2	14	52	2.802	100.0–1500.0	23	0.216	(12, 18, 25)
N_2	12	93	3.663	100.0–1500.0	34	0.086	(7, 12, 14)
O_2	14	117	3.402	100.0–1500.0	37	0.264	(5, 7, 8, 14, 25)
CO	16	115	3.566	80.0–1500.0	18	0.283	(13, 25)
CO_2	10	207	3.892	200.0–1500.0	22	0.358	(3, 5, 7, 25, 31)
Air	12	94	3.628	100.0–1500.0	18	0.316	(2, 7, 25, 31)
CH_4	12	157	3.700	100.0–1500.0	17	0.16	(7, 25)
C_3H_8	20	265	5.053	273.2– 463.2	16	0.118	(19, 26, 27, 29, 30)
n-C_5H_{12}	20	333	5.883	273.2– 492.3	12	0.185	(19, 28, 32)

[a] Standard error $= \left[\sum_{i}^{n} (\eta_{\text{calcd.}} - \eta_{\text{exptl}})^2/(n-1) \right]^{1/2}$.

Table V. Potential Parameters and Standard Errors for Lennard-Jones (6, 12) Potential Using Same Temperature Range and Same Data Points as Table III

Gas	ϵ/k, °K.	σ, A.	Standard Error
He	6.5	2.660	0.355
Ar	116.0	3.452	0.287
Ne	39.0	2.780	0.216
H_2	40.0	2.899	0.252
O_2	106.0	3.462	0.292
CO	91.0	3.702	0.420
CO_2	213.0	3.859	0.427
C_3H_8	254.0	5.021	0.143
n-C_5H_{12}	337.0	5.740	0.224

Table VI. Experimental and Calculated Values of Viscosity of n-Pentane as Function of Temperature

$(G.\ \text{cm.}^{-1}\ \text{sec.}^{-1} \times 10^6)$

T	η_{exptl}	L-J(6, 12)	L-J(6, 20)	Ref.
273.16	62.00	63.89	65.89	(19)
308.16	77.10	72.84	73.68	(19)
323.16	79.30	76.10	77.02	(19)
338.16	81.30	79.66	80.35	(19)
343.26	81.69	80.87	81.48	(32)
351.16	83.69	82.74	83.23	(19)
352.96	83.80	83.16	83.62	(19)
363.36	85.90	85.60	85.91	(19)
395.76	91.09	93.08	92.95	(29)
432.06	99.50	101.36	100.55	(28)
462.76	106.40	108.24	106.76	(28)
492.26	112.60	114.75	112.61	(28)
Standard error		0.224	0.185	
σ		5.740	5.883	
ϵ/k		337	333	

2. With an approximate value of ϵ/k, the value determined from the L-J (6, 12) potential, the reduced temperature was calculated.

3. The reduced collision integral $\Omega^{2,2*}$ (T^*) for the calculated reduced temperature was evaluated by using the Lagrangian four-point interpolation method.

4. Experimental viscosity data points at various temperatures and values of the reduced collision integral, $\Omega^{2,2*}(T^*)$, calculated in step 3, were substituted in Equation 23. Then the nonlinear least-square curve fitting program was used to evaluate the collision diameter, σ, for the entire temperature range.

5. Steps 2 through 5 were repeated with a successively adjusted new value of ϵ/k until the possible range of ϵ/k had been covered.

6. Steps 1 through 5 were repeated by changing the repulsive potential index, n, by an increment of 2 until the selected range of $n(8–20)$ had been covered.

From these results, a set of potential parameters, n, ϵ/k, and σ, which produced the best over-all fit to the experimental viscosity data with the smallest standard error of estimate, was chosen as the set of potential parameters for the gas.

The potential parameters for 12 gases—helium, argon, neon, hydrogen, nitrogen, oxygen, carbon monoxide, carbon dioxide, air, methane, propane, and n-pentane—are listed in Table IV along with their standard errors of estimate, number of data points, and the temperature range of data points used in the determination for each gas. For comparison, Table V lists these results obtained from the L-J (6, 12) potential for the same temperature range and the same number of data points. A representative calculation of the viscosity $vs.$ temperature using L-J (6, 12) and an improved L-J potential is presented in Table VI for n-pentane with the experimental data points.

ACKNOWLEDGMENT

NOMENCLATURE

A	=	quantity defined in Equation 15
A^*	=	ratio of collision integrals defined in Equation 5
B^*	=	ratio of collision integrals defined in Equation 6
b^*	=	reduced impact parameter
C^*	=	ratio of collision integrals defined in Equation 7
$E(r)$	=	intermolecular potential energy of interaction
E^*	=	ratio of collision integrals defined in Equation 8
$E^*(r^*)$	=	reduced intermolecular potential
F^*	=	ratio of collision integrals defined in Equation 9
f_η	=	correction factor for viscosity of a gas
f_λ	=	correction factor for thermal conductivity of a gas
f_D	=	correction factor for self-diffusion of a gas
g^{*2}	=	reduced relative kinetic energy of molecule
H	=	function defined in Equation 14
k	=	Boltzmann constant
l	=	constant
M	=	molecular weight
n	=	repulsive potential index

$Q^{l}(g^2)$ = collision cross sections of colliding molecules
$Q^{l*}(g^{*2})$ = reduced collision cross sections of colliding molecules
q = contributed from orbiting regions
r = intermolecular distance
r^* = reduced intermolecular distance
r_m = distance of closest approach at a given kinetic energy and impact parameter
r_m^* = reduced distance of closest approach at a given reduced kinetic energy and reduced impact parameter
r_{mo}^* = reduced distance of closest approach when $b^* = 0$
r_{mi}^* = reduced distance of closest approach when $b^* = g^{*2}$
r_n^* = distance of closest approach when $dE^*/dr^* = 0$ at $b^* = g^{*2}$
s = constant
T^* = reduced temperature
W_0 = quantity defined in Equation 18
W_k = quantity defined in Equation 19

Greek Letters

ϵ = maximum attraction of potential energy
η = viscosity
σ = collision diameter
χ = angle of deflection
$\Omega^{l,s,*}(T^*)$ = reduced collision integrals

LITERATURE CITED

(1) Amdur, I., *A.I.Ch.E. J.* 8, 521 (1962).
(2) Barker, J.A., Fock, W., Smith, F.J., *Phys. Fluids* 7, 897 (1964).
(3) Bearden, J.A., *Phys. Rev.* 56, 1023 (1939).
(4) Bernstein, R.B., *J. Chem. Phys.* 38, 515 (1963).
(5) Bonilla, C.F., Government Auxiliary Document AD-97581.
(6) Bonilla, C.F., Wang, S.J., Weiner, H., *Trans. ASME* 78, 967 (1954).
(7) Hilsenrath, J., Beckett, C.W., Benedict, W.S., Fano, L., Hoge, H.J., Masi, J.F., Nuttall, R.L., Touloukian, Y.S., Woolley, H.W., National Bureau of Standards, Circ. 564, 424 (1955).
(8) Hilsenrath, J., Touloukian, Y.S., *Trans. ASME* 76, (1954).

(9) Hirschfelder, J.O., Curtiss, C.F., Bird, R.B., "Molecular Theory of Gases and Liquids," Wiley, New York, 1964.
(10) Horton, G.K., Leech, J.W., *Phys. Soc. (London)* 82, 816 (1963).
(11) Itean, E.C., Gluck, A.R., Svelha, R.A., NASA Tech. Note D-481 (1961).
(12) Johnston, H.L., Grilly, E.R., *J. Phys. Chem.* 46, 948 (1942).
(13) Johnston, H.L., McCloskey, K.E., *Ibid.*, 44, 1038 (1940).
(14) Keyes, F.G., Project SQUID, Tech. Rept. 37.
(15) Kihara, T., *Rev. Mod. Phys.* 25, 831 (1953); 27, 412 (1955).
(16) Klein, M., National Bureau of Standards, Washington, D. C., private communication, 1968.
(17) Klein, M., Smith, F.J., Arnold Engineering Development Center, Tech. Rept. AEDC-TR-68-92.
(18) Kompaneets, V.Y., Rabot, S.N., *Leningrad Inst. Mekl. Khoz.* 9, 113 (1953).
(19) Lambert, J.D., Cotton, K.J., Pailthorpe, M.E., Robinson, M.E., Serivins, A.M., Vale, J., Young, R.M., *Proc. Roy. Soc. (London)* A231 (1955).
(20) Marquardt, D.L., *J. Soc. Ind. Appl. Math.* 2, 431 (1963).
(21) Mason, E.A., *J. Chem. Phys.* 22, 169 (1954).
(22) Monchick, L., Mason, E.A., *Ibid.*, 35, 1676 (1961).
(23) Mountain, R., Swanzig, R.W., *Ibid.*, 43, 4464 (1965).
(24) Rabinowitz, P., Weiss, G., *Math. Comp.* 13, 285 (1959).
(25) Rammler, E., Breitling, K., *Die Warme (Z. Dampfkessel Masschinenbetrieb)* 60, 620 (1937).
(26) Smith, A.S., Brown, G.G., *Ind. Eng. Chem.* 35, 705 (1943).
(27) Smith, F.J., Mason, E.A., Munn, R.J., *J. Chem. Phys.* 42, 1334 (1965).
(28) Titani, T., *Bull. Chem. Soc. (Japan)* 2, 161 (1927).
(29) *Ibid.*, 5, 98 (1930).
(30) Trautz, M., Zink, R., *Ann. Physik* 7, 427 (1930).
(31) Uchiyama, H., *Chem. Eng. (Japan)* 19(7), 342 (1955).
(32) Vasilesco, V., *Ann. Phys. (Paris)*, Ser. 11, 20, 292 (1945).