Appendix E

Tables for Prediction of Transport Properties

Table E.1 Lennard-Jones (6–12) Potential Parameters and Critical Properties

		Lennard-Jones parameters			Critical properties[g,h]				
Substance	Molecular Weight M	σ (Å)	ε/κ (K)	Ref.	T_c (K)	p_c (atm)	$\tilde{V}_c$ (cm^3/g-mole)	μ_c ($g/cm \cdot s \times 10^6$)	k_c ($cal/cm \cdot s \cdot K \times 10^6$)
Light elements:									
H_2	2.016	2.915	38.0	*a*	33.3	12.80	65.0	34.7	—
He	4.003	2.576	10.2	*a*	5.26	2.26	57.8	25.4	—
Noble gases:									
Ne	20.180	2.789	35.7	*a*	44.5	26.9	41.7	156.	79.2
Ar	39.948	3.432	122.4	*b*	150.7	48.0	75.2	264.	71.0
Kr	83.80	3.675	170.0	*b*	209.4	54.3	92.2	396.	49.4
Xe	131.29	4.009	234.7	*b*	289.8	58.0	118.8	490.	40.2
Simple polyatomic gases:									
Air	28.964[i]	3.617	97.0	*a*	132.4[i]	37.0[i]	86.7[i]	193.	90.8
N_2	28.013	3.667	99.8	*b*	126.2	33.5	90.1	180.	86.8
O_2	31.999	3.433	113.	*a*	154.4	49.7	74.4	250.	105.3
CO	28.010	3.590	110.	*a*	132.9	34.5	93.1	190.	86.5
CO_2	44.010	3.996	190.	*a*	304.2	72.8	94.1	343.	122.
NO	30.006	3.470	119.	*a*	180.	64.	57.	258.	118.2
N_2O	44.012	3.879	220.	*a*	309.7	71.7	96.3	332.	131.
SO_2	64.065	4.026	363.	*c*	430.7	77.8	122.	411.	98.6
F_2	37.997	3.653	112.	*a*	—	—	—	—	—
Cl_2	70.905	4.115	357.	*a*	417.	76.1	124.	420.	97.0
Br_2	159.808	4.268	520.	*a*	584.	102.	144.	—	—
I_2	253.809	4.982	550.	*a*	800.	—	—	—	—
Hydrocarbons:									
CH_4	16.04	3.780	154.	*b*	191.1	45.8	98.7	159.	158.
$CH{\equiv}CH$	26.04	4.114	212.	*d*	308.7	61.6	112.9	237.	—
$CH_2{=}CH_2$	28.05	4.228	216.	*b*	282.4	50.0	124.	215.	—
C_2H_6	30.07	4.388	232.	*b*	305.4	48.2	148.	210.	203.
$CH_3C{\equiv}CH$	40.06	4.742	261.	*d*	394.8	—	—	—	—
$CH_3CH{=}CH_2$	42.08	4.766	275.	*b*	365.0	45.5	181.	233.	—
C_3H_8	44.10	4.934	273.	*b*	369.8	41.9	200.	228.	—
n—C_4H_{10}	58.12	5.604	304.	*b*	425.2	37.5	255.	239.	—

i—C_4H_{10}	58.12	5.393	295.	*b*	408.1	36.0	263.	239.	—
n—C_5H_{12}	72.15	5.850	326.	*b*	469.5	33.2	311.	238.	—
i—C_5H_{12}	72.15	5.812	327.	*b*	460.4	33.7	306.	—	—
$C(CH_3)_4$	72.15	5.759	312.	*b*	433.8	31.6	303.	—	—
n—C_6H_{14}	86.18	6.264	342.	*b*	507.3	29.7	370.	248.	—
n—C_7H_{16}	100.20	6.663	352.	*b*	540.1	27.0	432.	254.	—
n—C_8H_{18}	114.23	7.035	361.	*b*	568.7	24.5	492	259.	—
n—C_9H_{20}	128.26	7.463	351.	*b*	594.6	22.6	548.	265.	—
Cyclohexane	84.16	6.143	313.	*d*	553.	40.0	308.	284.	—
Benzene	78.11	5.443	387.	*b*	562.6	48.6	260.	312.	—
Other organic compounds:									
CH_4	16.04	3.780	154.	*b*	191.1	45.8	98.7	159.	158.
CH_3Cl	50.49	4.151	355.	*c*	416.3	65.9	143.	338.	—
CH_2Cl_2	84.93	4.748	398.	*c*	510.	60.	—	—	—
$CHCl_3$	119.38	5.389	340.	*e*	536.6	54.	240.	410.	—
CCl_4	153.82	5.947	323.	*e*	556.4	45.0	276.	413.	—
C_2N_2	52.034	4.361	349.	*e*	400.	59.	—	—	—
COS	60.076	4.130	336.	*e*	378.	61.	—	—	—
CS_2	76.143	4.483	467.	*e*	552.	78.	170.	404.	—
CCl_2F_2	120.91	5.116	280.	*b*	384.7	39.6	218.	—	—

[a] J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids*, corrected printing with notes added, Wiley, New York (1964).

[b] L. S. Tee, S. Gotoh, and W. E. Stewart, *Ind. Eng. Chem. Fundamentals*, **5**, 356–363 (1966). The values for benzene are from viscosity data on that substance. The values for other substances are computed from Correlation (iii) of the paper.

[c] L. Monchick and E. A. Mason, *J. Chem. Phys.*, **35**, 1676–1697 (1961); parameters obtained from viscosity.

[d] L. W. Flynn and G. Thodos, *AIChE Journal*, **8**, 362–365 (1962); parameters obtained from viscosity.

[e] R. A. Svehla, *NASA Tech. Report R-132* (1962); parameters obtained from viscosity. This report provides extensive tables of Lennard-Jones parameters, heat capacities, and calculated transport properties.

[f] Values of the critical constants for the pure substances are selected from K. A. Kobe and R. E. Lynn, Jr., *Chem. Rev.*, **52**, 117–236 (1962); *Amer. Petroleum Inst. Research Proj.* **44**, Thermodynamics Research Center, Texas A&M University, College Station, Texas (1966); and *Thermodynamic Functions of Gases*, F. Din (editor), Vols. 1–3, Butterworths, London (1956, 1961, 1962).

[g] Values of the critical viscosity are from O. A. Hougen and K. M. Watson, *Chemical Process Principles*, Vol. 3, Wiley, New York (1947), p. 873.

[h] Values of the critical thermal conductivity are from E. J. Owens and G. Thodos, *AIChE Journal*, **3**, 454–461 (1957).

[i] For air, the molecular weight M and the pseudocritical properties have been computed from the average composition of dry air as given in COESA, *U.S. Standard Atmosphere 1976*, U.S. Government Printing Office, Washington, D.C. (1976).

Table E.2 Collision Integrals for Use with the Lennard-Jones (6–12) Potential for the Prediction of Transport Properties of Gases at Low Densities[a,b,c]

$\kappa T/\varepsilon$ or $\kappa T/\varepsilon_{AB}$	$\Omega_\mu = \Omega_k$ (for viscosity and thermal conductivity)	$\Omega_{\mathcal{D},AB}$ (for diffusivity)	$\kappa T/\varepsilon$ or $\kappa T/\varepsilon_{AB}$	$\Omega_\mu = \Omega_k$ (for viscosity and thermal conductivity)	$\Omega_{\mathcal{D},AB}$ (for diffusivity)
0.30	2.840	2.649	2.7	1.0691	0.9782
0.35	2.676	2.468	2.8	1.0583	0.9682
0.40	2.531	2.314	2.9	1.0482	0.9588
0.45	2.401	2.182	3.0	1.0388	0.9500
0.50	2.284	2.066	3.1	1.0300	0.9418
0.55	2.178	1.965	3.2	1.0217	0.9340
0.60	2.084	1.877	3.3	1.0139	0.9267
0.65	1.999	1.799	3.4	1.0066	0.9197
0.70	1.922	1.729	3.5	0.9996	0.9131
0.75	1.853	1.667	3.6	0.9931	0.9068
0.80	1.790	1.612	3.7	0.9868	0.9008
0.85	1.734	1.562	3.8	0.9809	0.8952
0.90	1.682	1.517	3.9	0.9753	0.8897
0.95	1.636	1.477	4.0	0.9699	0.8845
1.00	1.593	1.440	4.1	0.9647	0.8796
1.05	1.554	1.406	4.2	0.9598	0.8748
1.10	1.518	1.375	4.3	0.9551	0.8703
1.15	1.485	1.347	4.4	0.9506	0.8659
1.20	1.455	1.320	4.5	0.9462	0.8617
1.25	1.427	1.296	4.6	0.9420	0.8576
1.30	1.401	1.274	4.7	0.9380	0.8537
1.35	1.377	1.253	4.8	0.9341	0.8499
1.40	1.355	1.234	4.9	0.9304	0.8463
1.45	1.334	1.216	5.0	0.9268	0.8428
1.50	1.315	1.199	6.0	0.8962	0.8129
1.55	1.297	1.183	7.0	0.8727	0.7898
1.60	1.280	1.168	8.0	0.8538	0.7711
1.65	1.264	1.154	9.0	0.8380	0.7555
1.70	1.249	1.141	10.0	0.8244	0.7422
1.75	1.235	1.128	12.0	0.8018	0.7202
1.80	1.222	1.117	14.0	0.7836	0.7025
1.85	1.209	1.105	16.0	0.7683	0.6878
1.90	1.198	1.095	18.0	0.7552	0.6751
1.95	1.186	1.085	20.0	0.7436	0.6640
2.00	1.176	1.075	25.0	0.7198	0.6414
2.10	1.156	1.058	30.0	0.7010	0.6235
2.20	1.138	1.042	35.0	0.6854	0.6088
2.30	1.122	1.027	40.0	0.6723	0.5964
2.40	1.107	1.013	50.0	0.6510	0.5763
2.50	1.0933	1.0006	75.0	0.6140	0.5415
2.60	1.0807	0.9890	100.0	0.5887	0.5180

[a] The values in this table, applicable for the Lennard-Jones (6–12) potential, are interpolated from the results of L. Monchick and E. A. Mason, *J. Chem. Phys.*, **35**, 1676–1697 (1961). The Monchick–Mason table is believed to be slightly better than the earlier table by J. O. Hirschfelder, R. B. Bird, and E. L. Spotz, *J. Chem. Phys.*, **16**, 968–981 (1948).

[b] This table has been extended to lower temperatures by C. F. Curtiss, *J. Chem. Phys.*, **97**, 7679–7686 (1992). Curtiss showed that at low temperatures, the Boltzmann equation needs to be modified to take into account "orbiting pairs" of molecules. Only by making this modification is it possible to get a smooth transition from quantum to classical behavior. The deviations are appreciable below dimensionless temperatures of 0.30.

[c] The collision integrals have been curve-fitted by P. D. Neufeld, A. R. Jansen, and R. A. Aziz, *J. Chem. Phys.*, **57**, 1100–1102 (1972), as follows:

$$\Omega_\mu = \Omega_k = \frac{1.16145}{T^{*0.14874}} + \frac{0.52487}{\exp(0.77320T^*)} + \frac{2.16178}{\exp(2.43787T^*)} \tag{E.2-1}$$

$$\Omega_{\mathcal{D},AB} = \frac{1.06036}{T^{*0.15610}} + \frac{0.19300}{\exp(0.47635T^*)} + \frac{1.03587}{\exp(1.52996T^*)} + \frac{1.76474}{\exp(3.89411T^*)} \tag{E.2-2}$$

where $T^* = \kappa T/\varepsilon$.