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Appendix J

Mass-Transfer Diffusion Coefficients in Binary Systems

Table J.1 Binary Mass Diffusivities in Gases*

System	T, K	$D_{AB}P$, cm^2 atm/s	$D_{AB}P$, m^2 Pa/s
Air			
Ammonia	273	0.198	2.006
Aniline	298	0.0726	0.735
Benzene	298	0.0962	0.974
Bromine	293	0.091	0.923
Carbon dioxide	273	0.136	1.378
Carbon disulfide	273	0.0883	0.894
Chlorine	273	0.124	1.256
Diphenyl	491	0.160	1.621
Ethyl acetate	273	0.0709	0.718
Ethanol	298	0.132	1.337
Ethyl ether	293	0.0896	0.908
Iodine	298	0.0834	0.845
Methanol	298	0.162	1.641
Mercury	614	0.473	4.791
Naphthalene	298	0.0611	0.619
Nitrobenzene	298	0.0868	0.879
n-Octane	298	0.0602	0.610
Oxygen	273	0.175	1.773
Propyl acetate	315	0.092	0.932
Sulfur dioxide	273	0.122	1.236
Toluene	298	0.0844	0.855
Water	298	0.260	2.634
Ammonia			
Ethylene	293	0.177	1.793
Argon			
Neon	293	0.329	3.333
Carbon dioxide			
Benzene	318	0.0715	0.724
Carbon disulfide	318	0.0715	0.724
Ethyl acetate	319	0.0666	0.675

(continued)

Table J.1 *(continued)*

System	T, K	$D_{AB}P$, cm^2 atm/s	$D_{AB}P$, m^2 Pa/s
Carbon dioxide			
Ethanol	273	0.0693	0.702
Ethyl ether	273	0.0541	0.548
Hydrogen	273	0.550	5.572
Methane	273	0.153	1.550
Methanol	298.6	0.105	1.064
Nitrogen	298	0.165	1.672
Nitrous oxide	298	0.117	1.185
Propane	298	0.0863	0.874
Water	298	0.164	1.661
Carbon monoxide			
Ethylene	273	0.151	1.530
Hydrogen	273	0.651	6.595
Nitrogen	288	0.192	1.945
Oxygen	273	0.185	1.874
Helium			
Argon	273	0.641	6.493
Benzene	298	0.384	3.890
Ethanol	298	0.494	5.004
Hydrogen	293	1.64	16.613
Neon	293	1.23	12.460
Water	298	0.908	9.198
Hydrogen			
Ammonia	293	0.849	8.600
Argon	293	0.770	7.800
Benzene	273	0.317	3.211
Ethane	273	0.439	4.447
Methane	273	0.625	6.331
Oxygen	273	0.697	7.061
Water	293	0.850	8.611
Nitrogen			
Ammonia	293	0.241	2.441
Ethylene	298	0.163	1.651
Hydrogen	288	0.743	7.527
Iodine	273	0.070	0.709
Oxygen	273	0.181	1.834
Oxygen			
Ammonia	293	0.253	2.563
Benzene	296	0.0939	0.951
Ethylene	293	0.182	1.844

* R. C. Reid and T. K. Sherwood, *The Properties of Gases and Liquids*, McGraw-Hill Book Company, New York, 1958, Chap. 8.

Table J.2 Binary Mass Diffusivities in Liquids*

Solute *A*	Solvent *B*	Temperature, in K	Solute Concentration, in g mole/liter or kg mole/m^3	Diffusivity cm^2/s $\times$ 10^5 or m^2/s $\times$ 10^9
Chlorine	Water	289	0.12	1.26
Hydrogen chloride	Water	273	9	2.7
			2	1.8
		283	9	3.3
			2.5	2.5
		289	0.5	2.44
Ammonia	Water	278	3.5	1.24
		288	1.0	1.77
Carbon dioxide	Water	283	0	1.46
		293	0	1.77
Sodium chloride	Water	291	0.05	1.26
			0.2	1.21
			1.0	1.24
			3.0	1.36
			5.4	1.54
Methanol	Water	288	0	1.28
Acetic acid	Water	285.5	1.0	0.82
			0.01	0.91
		291	1.0	0.96
Ethanol	Water	283	3.75	0.50
			0.05	0.83
		289	2.0	0.90
n-Butanol	Water	288	0	0.77
Carbon dioxide	Ethanol	290	0	3.2
Chloroform	Ethanol	293	2.0	1.25

* R. E. Treybal, *Mass Transfer Operations,* McGraw-Hill Book Company, New York, 1955, p. 25.

Table J.3 Binary Diffusivities in Solids*

Solute	Solid	K	Diffusivity, cm^2/s or m^2/s $\times$ 10^4	Diffusivity, ft^2/hr
Helium	Pyrex	293	4.49×10^{-11}	1.74×10^{-10}
		773	2.00×10^{-8}	7.76×10^{-8}
Hydrogen	Nickel	358	1.16×10^{-8}	4.5×10^{-8}
		438	1.05×10^{-7}	4.07×10^{-7}
Bismuth	Lead	293	1.10×10^{-16}	4.27×10^{-16}
Mercury	Lead	293	2.50×10^{-15}	9.7×10^{-15}
Antimony	Silver	293	3.51×10^{-21}	1.36×10^{-20}
Aluminum	Copper	293	1.30×10^{-30}	5.04×10^{-30}
Cadmium	Copper	293	2.71×10^{-15}	1.05×10^{-14}

* R. M. Barrer, *Diffusion In and Through Solids,* The Macmillan Company, New York, 1941.

Table 24.4 Molecular Volumes at Normal Boiling Point for Some Commonly Encountered Compounds

Compound	Molecular volume, cm^3/g mole	Compound	Molecular volume, in cm^3/g mole
Hydrogen, H_2	14.3	Nitric oxide, NO	23.6
Oxygen, O_2	25.6	Nitrous oxide, N_2O	36.4
Nitrogen, N_2	31.2	Ammonia, NH_3	25.8
Air	29.9	Water, H_2O	18.9
Carbon monoxide, CO	30.7	Hydrogen sulfide, H_2S	32.9
Carbon dioxide, CO_2	34.0	Bromine, Br_2	53.2
Carbonyl sulfide, COS	51.5	Chlorine, Cl_2	48.4
Sulfur dioxide, SO_2	44.8	Iodine, I_2	71.5

Table 24.5 Atomic Volumes for Complex Molecular Volumes for Simple Substances†

Element	Atomic volume, in cm^3/g mole	Element	Atomic volume, in cm^3/g mole
Bromine	27.0	Oxygen, except as noted below	7.4
Carbon	14.8	Oxygen, in methyl esters	9.1
Chlorine	21.6	Oxygen, in methyl ethers	9.9
Hydrogen	3.7	Oxygen, in higher ethers and other esters	11.0
Iodine	37.0	Oxygen, in acids	12.0
Nitrogen, double bond	15.6	Sulfur	25.6
Nitrogen, in primary amines	10.5		
Nitrogen, in secondary amines	12.0		

† G. Le Bas, *The Molecular Volumes of Liquid Chemical Compounds,* Longmans, Green & Company, Ltd., London, 1915.

Solvent	Φ_B
water	2.26*
methanol	1.9
ethanol	1.5
benzene, ether, heptane, and other unassociated solvents	1.0

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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)	$\mu_c \times 10^6$ (g/cm · s)	$k_c \times 10^6$ (cal/cm · s · K)
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)	$\Omega_{\mathfrak{D},AB}$ (for diffusivity)	$\kappa T/\varepsilon$ or $\kappa T/\varepsilon_{AB}$	$\Omega_\mu = \Omega_k$ (for viscosity and thermal conductivity)	$\Omega_{\mathfrak{D},AB}$ (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. Janzen, and R. A. Aziz, *J. Chem. Phys.*, **57**, 1100–1102 (1972), as follows:

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

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

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