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TABLE 2-1. ATOMIC AND MOLECULAR VOLUMES AT THE NORMAL BOILING POINT (TREYBAL, 1968)

	Atomic Volume × 10^3 *($m^3/kgatom$)*		*Molecular Volume* × 10^3 *($m^3/kgmol$)*
Bromine	27.0	Air	29.9
Carbon	14.8	Br_2	53.2
Chlorine	24.6	Cl_2	48.4
Hydrogen	3.7	CO	30.7
Iodine	37.0	CO_2	34.0
Nitrogen	15.6	COS	51.5
Nitrogen in primary amines	10.5	H_2	14.3
Nitrogen in secondary amines	12.0	H_2O	18.9
Oxygen	7.4	H_2S	32.9
Oxygen in methyl esters	9.1	I_2	71.5
Oxygen in higher esters	11.0	N_2	31.2
Oxygen in acids	12.0	NH_3	25.8
Oxygen in methyl ethers	9.9	NO	23.6
Oxygen in higher ethers	11.0	N_2O	36.4
Sulfur	25.6	O_2	25.6
Benzene ring	−15.0	SO_2	44.8
Naphthalene ring	−30.0		

TABLE 2-2. ATOMIC AND MOLECULAR DIFFUSION VOLUMES FOR THE EQUATION OF FULLER ET AL. (1966)[a]

Atomic and Structural Diffusion Volume Increments, v × 10^3 ($m^3/kgatom$)			
C	16.5	(Cl)	19.5
H	1.98	(S)	17.0
O	5.48	Aromatic ring	−20.2
(N)	5.69	Heterocyclic ring	−20.2
H_2	7.07	CO	18.9
D_2	6.70	CO_2	26.9
He	2.88	N_2O	35.9
N_2	17.9	NH_3	14.9
O_2	16.6	H_2O	12.7
Air	20.1	(CCl_2F_2)	114.8
Ar	16.1	(SF_6)	69.7
Kr	22.8	(Cl_2)	37.7
(Xe)	37.9	(Br_2)	67.2
Ne	5.59	(SO_2)	41.1

[a]Parentheses indicate that the value listed is based on only a few data points.

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TABLE 2-3. COLLISION DIAMETERS AND ENERGY PARAMETERS FOR THE LENNARD-JONES EQUATION (SVEHLA, 1962)

Molecule	*Compound*	$\sigma \times 10^{10}$ (*m*)	ϵ/k (*K*)
Ar	Argon	3.542	93.3
He	Helium	2.551	10.22
Kr	Krypton	3.655	178.9
Ne	Neon	2.820	32.8
Xe	Xenon	4.047	1.0
Air	Air	3.711	78.6
AsH_3	Arsine	4.145	259.8
BCl_3	Boron chloride	5.127	337.7
BF_3	Boron fluoride	4.198	186.3
$B(OCH_3)_3$	Methyl borate	5.503	396.7
Br_2	Bromine	4.296	507.9
CCl_4	Carbon tetrachloride	5.947	322.7
CF_4	Carbon tetrafluoride	4.662	134.0
$CHCl_3$	Chloroform	5.389	340.2
CH_2Cl_2	Methylene chloride	4.898	356.3
CH_3Br	Methyl bromide	4.118	449.2
CH_3Cl	Methyl chloride	4.182	350
CH_3OH	Methanol	3.626	481.8
CH_4	Methane	3.758	148.6
CO	Carbon monoxide	3.690	91.7
COS	Carbonyl sulfide	4.130	336.0
CO_2	Carbon dioxide	3.941	195.2
CS_2	Carbon disulfide	4.483	467
C_2H_2	Acetylene	4.033	231.8
C_2H_4	Ethylene	4.163	224.7
C_2H_6	Ethane	4.443	215.7
C_2H_5Cl	Ethyl chloride	4.898	300

$$D_{AB} = K' \frac{T^{3/2}}{P A_{avg}} \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^{1/2} \quad \text{Eq. 2-5}$$

Hirschfelder: $K' = 1.858 \times 10^{-27}$

$A_{avg} = \sigma_{AB}^2 \Omega_D$; $\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2}$

Ω_D from Table 2-4 (need ϵ from Table 2-3

TABLE 2-3. (CONTINUED)

Molecule	*Compound*	$\sigma \times 10^{10}$ (*m*)	ϵ/k (*K*)
C_2H_5OH	Ethanol	4.530	362.6
C_2N_2	Cyanogen	4.361	348.6
CH_3OCH_3	Methyl ether	4.307	395.0
CH_2CHCH_3	Propylene	4.678	298.9
CH_3CCH	Methylacetylene	4.761	251.8
C_3H_6	Cyclopropane	4.807	248.9
C_3H_8	Propane	5.118	237.1
n-C_3H_7OH	*n*-Propyl alcohol	4.549	576.7
CH_3COCH_3	Acetone	4.600	560.2
CH_3COOCH_3	Methyl acetate	4.936	469.8
n-C_4H_{10}	*n*-Butane	4.687	531.4
i-C_4H_{10}	Isobutane	5.278	330.1
$C_2H_5OC_2H_5$	Ethyl ether	5.678	313.8
$CH_3COOC_2H_5$	Ethyl acetate	5.205	521.3
n-C_5H_{12}	*n*-Pentane	5.784	341.1
$C(CH_3)_4$	2,2-Dimethylpropane	6.464	193.4
C_6H_6	Benzene	5.349	412.3
C_6H_{12}	Cyclohexane	6.182	297.1
n-C_6H_{14}	*n*-Hexane	5.949	399.3
Cl_2	Chlorine	4.217	316.0
F_2	Fluorine	3.357	112.6
HBr	Hydrogen bromide	3.353	449
HCN	Hydrogen cyanide	3.630	569.1
HCl	Hydrogen chloride	3.339	344.7
HF	Hydrogen fluoride	3.148	330
HI	Hydrogen iodide	4.211	288.7
H_2	Hydrogen	2.827	59.7
H_2O	Water	2.641	809.1
H_2O_2	Hydrogen peroxide	4.196	289.3
H_2S	Hydrogen sulfide	3.623	301.1
Hg	Mercury	2.969	750
$HgBr_2$	Mercuric bromide	5.080	686.2
$HgCl_2$	Mercuric chloride	4.550	750
HgI_2	Mercuric iodide	5.625	695.6
I_2	Iodine	5.160	474.2
NH_3	Ammonia	2.900	558.3
NO	Nitric oxide	3.492	116.7
NOCl	Nitrosyl chloride	4.112	395.3
N_2	Nitrogen	3.798	71.4
N_2O	Nitrous oxide	3.828	232.4
O_2	Oxygen	3.467	106.7
PH_3	Phosphine	3.981	251.5
SF_6	Sulfur hexafluoride	5.128	222.1
SO_2	Sulfur dioxide	4.112	335.4
SiF_4	Silicon tetrafluoride	4.880	171.9
SiH_4	Silicon hydride	4.084	207.6
$SnBr_4$	Stannic bromide	6.388	563.7
UF_6	Uranium hexafluoride	5.967	236.8

Determine D_{AB,T_2,P_2} from D_{AB,T_1,P_1}

- calculate $\frac{kT_1}{\epsilon}$ and $\frac{kT_2}{\epsilon}$ $\underset{\text{Table 2-4}}{\Rightarrow}$ Ω_{T_1} and Ω_{T_2}

TABLE 2-4. VALUES OF THE COLLISION INTEGRAL Ω_D BASED ON THE LENNARD-JONES POTENTIAL (HIRSCHFELDER ET AL., 1954[a])

kT/ϵ	Ω_D	kT/ϵ	Ω_D	kT/ϵ	Ω_D
0.30	2.662	1.65	1.153	4.0	0.8836
0.35	2.476	1.70	1.140	4.1	0.8788
0.40	2.318	1.75	1.128	4.2	0.8740
0.45	2.184	1.80	1.116	4.3	0.8694
0.50	2.066	1.85	1.105	4.4	0.8652
0.55	1.966	1.90	1.094	4.5	0.8610
0.60	1.877	1.95	1.084	4.6	0.8568
0.65	1.798	2.00	1.075	4.7	0.8530
0.70	1.729	2.1	1.057	4.8	0.8492
0.75	1.667	2.2	1.041	4.9	0.8456
0.80	1.612	2.3	1.026	5.0	0.8422
0.85	1.562	2.4	1.012	6	0.8124
0.90	1.517	2.5	0.9996	7	0.7896
0.95	1.476	2.6	0.9878	8	0.7712
1.00	1.439	2.7	0.9770	9	0.7556
1.05	1.406	2.8	0.9672	10	0.7424
1.10	1.375	2.9	0.9576	20	0.6640
1.15	1.346	3.0	0.9490	30	0.6232
1.20	1.320	3.1	0.9406	40	0.5960
1.25	1.296	3.2	0.9328	50	0.5756
1.30	1.273	3.3	0.9256	60	0.5596
1.35	1.253	3.4	0.9186	70	0.5464
1.40	1.233	3.5	0.9120	80	0.5352
1.45	1.215	3.6	0.9058	90	0.5256
1.50	1.198	3.7	0.8998	100	0.5130
1.55	1.182	3.8	0.8942	200	0.4644
1.60	1.167	3.9	0.8888	400	0.4170

[a] Hirschfelder et al. use the symbols T^* for kT/ϵ and $\Omega^{(1,1)*}$ for Ω_D.

$$D_{AB,T_2,P_2} = D_{AB,T_1,P_1} \frac{P_1}{P_2} \left(\frac{T_2}{T_1}\right)^{3/2} \frac{\Omega_{T_1}}{\Omega_{T_2}}$$

TABLE 2-5. INTERDIFFUSION COEFFICIENTS FOR BINARY GASES AT 1 ATM PRESSURE (101.325 KPA) (MARRERO AND MASON, 1972)

System	$T(K)$	$D_{AB} \times 10^4$ (m^2/s)
Air–carbon dioxide	317.2	0.177
Air–ethanol	313	0.145
Air–helium	317.2	0.765
Air–*n*-hexane	328	0.093
Air–*n*-pentane	294	0.071
Air–water	313	0.288
Argon–ammonia	333	0.253
Argon–carbon dioxide	276.2	0.133
Argon–helium	298	0.729
Argon–hydrogen	242.2	0.562
	448	1.76
	806	4.86
	1069	8.10
Argon–methane	298	0.202
Argon–sulfur dioxide	263	0.077
Carbon dioxide–helium	298	0.612
Carbon dioxide–nitrogen	298	0.167
Carbon dioxide–nitrous oxide	312.8	0.128
Carbon dioxide–oxygen	293.2	0.153
Carbon dioxide–sulfur dioxide	263	0.064
Carbon dioxide–water	307.2	0.198
	352.3	0.245
Carbon monoxide–nitrogen	373	0.318
Helium–benzene	423	0.610
Helium–ethanol	423	0.821
Helium–methane	298	0.675
Helium–methanol	423	1.032
Helium–nitrogen	298	0.687
Helium–oxygen	298	0.729
Helium–*i*-propanol	423	0.677
Helium–water	307.1	0.902
Hydrogen–acetone	296	0.424
Hydrogen–ammonia	298	0.783
	358	1.093
	473	1.86
	533	2.149
Hydrogen–benzene	311.3	0.404
Hydrogen–cyclohexane	288.6	0.319
Hydrogen–methane	288	0.694
Hydrogen–nitrogen	298	0.784
	573	2.147
Hydrogen–sulfur dioxide	473	1.23
Hydrogen–thiophene	302	0.400
Hydrogen–water	328.5	1.121
Methane–water	352.3	0.356
Nitrogen–ammonia	298	0.230
	358	0.328
Nitrogen–benzene	311.3	0.102
Nitrogen–cyclohexane	288.6	0.0731
Nitrogen–sulfur dioxide	263	0.104
Nitrogen–water	307.5	0.256
	352.1	0.359
Oxygen–benzene	311.3	0.101
Oxygen–carbon tetrachloride	296	0.0749
Oxygen–cyclohexane	288.6	0.0746
Oxygen–water	352.3	0.352

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TABLE 2-6. EXPERIMENTAL DIFFUSION COEFFICIENTS AT INFINITE DILUTION (SHERWOOD ET AL., 1975)

Solute A	*Solvent B*	*T(K)*	$D^{\circ}_{AB} \times 10^9$ (m^2/s)
Acetic acid	Acetone	298	3.31
Benzoic acid	Acetone	298	2.62
Carbon dioxide	Amyl alcohol	298	1.91
Water	Aniline	293	0.70
Acetic acid	Benzene	298	2.09
Carbon tetrachloride	Benzene	298	1.92
Cinnamic acid	Benzene	298	1.12
Ethanol	Benzene	280.6	1.77
Ethylene chloride	Benzene	288	2.25
Methanol	Benzene	298	3.82
Napthalene	Benzene	280.6	1.19
Carbon dioxide	*i*-Butanol	298	2.20
Acetone	Carbon tetrachloride	293	1.86
Benzene	Chlorobenzene	293	1.25
Acetone	Chloroform	288	2.36
Benzene	Chloroform	288	2.51
Ethanol	Chloroform	288	2.20
Carbon tetrachloride	Cyclohexane	298	1.49
Azobenzene	Ethanol	293	0.74
Camphor	Ethanol	293	0.70
Carbon dioxide	Ethanol	290	3.20
Carbon dioxide	Ethanol	298	3.42
Glycerol	Ethanol	293	0.51
Pyridine	Ethanol	293	1.10
Urea	Ethanol	285	0.54
Water	Ethanol	298	1.132
Water	Ethylene glycol	293	0.18
Water	Glycerol	293	0.0083
Carbon dioxide	Heptane	298	6.03
Carbon tetrachloride	*n*-Hexane	298	3.70
Toluene	*n*-Hexane	298	4.21
Carbon dioxide	Kerosene	298	2.50
Tin	Mercury	303	1.60
Water	*n*-Propanol	288	0.87
Water	1,2-Propylene glycol	293	0.0075
Acetic acid	Toluene	298	2.26
Acetone	Toluene	293	2.93
Benzoic acid	Toluene	293	1.74
Chlorobenzene	Toluene	293	2.06
Ethanol	Toluene	288	3.00
Carbon dioxide	White spirit	298	2.11

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TABLE 6.5-1. *Diffusivities and Permeabilities in Solids*

Solute (A)	Solid (B)	T (K)	D_{AB}, Diffusion Coefficient [m^2/s]	Solubility, S $\left[\frac{m^3\ solute(STP)}{m^3\ solid \cdot atm}\right]$	Permeability, P_M $\left[\frac{m^3\ solute(STP)}{s \cdot m^2 \cdot atm/m}\right]$
H_2	Vulcanized rubber	298	$0.85(10^{-9})$	0.040	$0.342(10^{-10})$
O_2		298	$0.21(10^{-9})$	0.070	$0.152(10^{-10})$
N_2		298	$0.15(10^{-9})$	0.035	$0.054(10^{-10})$
CO_2		298	$0.11(10^{-9})$	0.90	$1.01(10^{-10})$
H_2	Vulcanized neoprene	290	$0.103(10^{-9})$	0.051	
		300	$0.180(10^{-9})$	0.053	
H_2	Polyethylene	298			$6.53(10^{-12})$
O_2		303			$4.17(10^{-12})$
N_2		303			$1.52(10^{-12})$
O_2	Nylon	303			$0.029(10^{-12})$
N_2		303			$0.0152(10^{-12})$
Air	English leather	298			$0.15-0.68 \times 10^{-4}$
H_2O	Wax	306			$0.16(10^{-10})$
H_2O	Cellophane	311			$0.91-1.82(10^{-10})$
He	Pyrex glass	293			$4.86(10^{-15})$
		373			$20.1(10^{-15})$
He	SiO_2	293	$2.4-5.5(10^{-14})$	0.01	
H_2	Fe	293	$2.59(10^{-13})$		
Al	Cu	293	$1.3(10^{-34})$		

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TABLE 6.5-1. *Diffusivities and Permeabilities in Solids*

Solute (*A*)	Solid (*B*)	*T* (*K*)	D_{AB}, Diffusion Coefficient [m^2/s]	Solubility, *S* $\left[\frac{m^3\ solute(STP)}{m^3\ solid \cdot atm}\right]$	Permeability, P_M $\left[\frac{m^3\ solute(STP)}{s \cdot m^2 \cdot atm/m}\right]$
H_2	Vulcanized rubber	298	$0.85(10^{-9})$	0.040	$0.342(10^{-10})$
O_2		298	$0.21(10^{-9})$	0.070	$0.152(10^{-10})$
N_2		298	$0.15(10^{-9})$	0.035	$0.054(10^{-10})$
CO_2		298	$0.11(10^{-9})$	0.90	$1.01(10^{-10})$
H_2	Vulcanized neoprene	290	$0.103(10^{-9})$	0.051	
		300	$0.180(10^{-9})$	0.053	
H_2	Polyethylene	298			$6.53(10^{-12})$
O_2		303			$4.17(10^{-12})$
N_2		303			$1.52(10^{-12})$
O_2	Nylon	303			$0.029(10^{-12})$
N_2		303			$0.0152(10^{-12})$
Air	English leather	298			$0.15-0.68 \times 10^{-4}$
H_2O	Wax	306			$0.16(10^{-10})$
H_2O	Cellophane	311			$0.91-1.82(10^{-10})$
He	Pyrex glass	293			$4.86(10^{-15})$
		373			$20.1(10^{-15})$
He	SiO_2	293	$2.4-5.5(10^{-14})$	0.01	
H_2	Fe	293	$2.59(10^{-13})$		
Al	Cu	293	$1.3(10^{-34})$		