

Appendix E

Data

Table E.1 Lennard-Jones parameters ε and σ for several molecules from simulations.^{a)}

Compound	(ε/k) (K)	σ (10^{-12} m)	Compound	(ε/k) (K)	σ (10^{-12} m)
Ar	111.84	362.3	CH ₄	140.42	401.5
Kr	154.87	389.5	CD ₄	138.16	402.3
Xe	213.96	426.0	C ₂ H ₆	216.12	478.2
O ₂	113.27	365.4	<i>n</i> C ₃ H ₈	255.18	547.1
N ₂	91.85	391.9	<i>n</i> C ₄ H ₁₀	287.20	608.1
F ₂	104.29	357.1	<i>n</i> C ₅ H ₁₂	309.75	670.9
Cl ₂	296.27	448.5	<i>n</i> C ₆ H ₁₄	327.47	731.9
CF ₄	155.31	491.1	<i>n</i> C ₇ H ₁₆	340.97	790.2
CCl ₄	378.86	624.1	<i>c</i> C ₃ H ₆	277.46	509.2
SiH ₄	193.65	453.9	<i>c</i> C ₅ H ₁₀	346.11	610.0
SiF ₄	140.14	669.2	C ₆ H ₆	377.46	617.4
SiCl ₄	338.01	668.2	C ₂ H ₂	209.11	463.5
TiCl ₄	417.49	672.5	C ₂ H ₄	200.78	458.9
SF ₆	206.85	578.3	CO ₂	201.71	444.4
UF ₆	323.61	637.9	CS ₂	388.81	498.3

- a) Data from Ref. [1], obtained from fitting MD simulation results of the pressure at low density and the Soave equation of state.

Table E.2 Lennard-Jones parameters ε and σ for several molecules from experimental data.^{a)}

Compound	(ε/k) (K)	σ (10^{-12} m)	Compound	(ε/k) (K)	σ (10^{-12} m)
Ne	35.60	274.9	CH ₄	148.2 (137*)	381.7 (382.2*)
Ar	119.8	340.5	C ₂ H ₆	230*	441.8*
Kr	171	360	<i>n</i> C ₃ H ₈	254*	506.1*
Xe	221	410	<i>n</i> C ₄ H ₁₀	410*	499.7*
O ₂	117.5	358	<i>n</i> C ₅ H ₁₂	345*	576.9*
N ₂	95.05	369.8	<i>n</i> C ₆ H ₁₄	413*	590.9*
F ₂	112*	365.3	CH ₃ OH	507*	358.5*
Cl ₂	357*	411.5*	C ₂ H ₅ OH	391*	445.5*
Br ₂	520*	426.8*	C ₆ H ₆	440*	527*
I ₂	550*	498.2*	C ₂ H ₂	185*	422.1*
CH ₃ Cl	855	337.5	C ₂ H ₄	205*	423.2*
CH ₂ Cl ₂	406	475.9	CO ₂	189	448.6
CHCl ₃	327	543.0	CS ₂	488*	443.8*
CCl ₄	327*	588.1*	SiF ₄	149	559
CF ₄	152.5	470	SF ₆	200.9	551

a) Data from Ref. [2], obtained from the viscosity (*) or from the second virial coefficient.

Table E.3 Thermodynamic vapor pressure constants a , b , and c for several compounds.^{a)}

Molecule	a	b	c	L_0 (cal · mol ⁻¹)
Ar	14.059	2.814	498	2278
CS ₂	15.9206	2.90	1844	8444
H ₂ O	20.9586 (17.443)	4.0843 (3.868)	2825.3 (2795)	12926 (13611)
H ₂ S	11.778	1.510	1145	5248
NH ₃	17.718	3.406	1612.5	7377
CH ₄	14.9640	3.283	598.4	2739
CH ₃ Cl	22.0114	5.133	1701	7786
CH ₂ Cl ₂	20.2795	4.2857	2098.1	9601
CHCl ₃	12.2999	3.9158	2179.1	9974
CCl ₄	24.3085	5.669	2452.6	11220
C ₂ H ₆	16.1506	3.332	1055	4831
<i>n</i> C ₃ H ₈	15.772	3.003	1325	6066
<i>n</i> C ₄ H ₁₀	19.877	4.376	1729	7912
<i>n</i> C ₅ H ₁₂	22.752	5.253	2099	9611
<i>n</i> C ₆ H ₁₄	25.281	6.013	2465	11284
<i>n</i> C ₈ H ₁₈	30.040	7.396	3162	14473
CH ₃ OH	22.43	4.634	2661	12180
<i>n</i> C ₄ H ₉ OH	40.21	10.35	4100	18750
<i>n</i> C ₅ H ₁₁ OH	46.49	12.42	4580	20940
<i>n</i> C ₆ H ₁₃ OH	51.00	13.80	5068	23170
<i>n</i> C ₇ H ₁₅ OH	56.20	15.41	5580	25510
<i>n</i> C ₈ H ₁₇ OH	65.21	18.40	6190	28300
C ₆ H ₆	20.818 (26.075)	4.7793 (6.203)	2388 (2610)	10927 (11940)
(CH ₃) ₃ N	30.094	7.978	2142	10030
C ₆ H ₅ COOH	30.172	6.720	4714	21567
(CH ₃) ₃ CO	19.557	3.966	2203	10078

$\log P_{\text{sat}}$ (mmHg) = $a - b \log T - c/T$, where T [K] and $L_0 = 2.303Rc$ with R the gas constant.

a) Data from Ref. [3].

Table E.4 Trouton constant C for several molecules.^{a)}

Molecule	C	Molecule	C	Molecule	C
Ar	9.0	CH ₄	8.8	H ₂ S	10.6
Kr	9.1	C ₂ H ₆	9.6	SO ₂	11.4
Xe	9.2	n-C ₄ H ₁₀	9.9	CH ₃ Cl	10.4
Rn	9.4	i-C ₄ H ₁₀	9.8	CHCl ₃	10.6
N ₂	8.7	n-C ₇ H ₁₆	10.3	(CH ₃) ₂ O	10.4
O ₂	9.1	c-C ₆ H ₁₂	10.2	NH ₃	11.7
Cl ₂	10.3	C ₆ H ₆	10.5	H ₂ O	13.1
CO	8.9	HCl	10.3	CH ₃ OH	12.6
N ₂ O	10.8	HBr	10.3	C ₂ H ₅ OH	13.2

a) Data from Ref. [4].

Table E.5 Vogel constants A , B , and C for the viscosity η of some polar liquids.^{a)}

	$-A$ (Pa s)	B (°C)	$-C$ (°C)	% error	T -range (°C)
Ammonia	1.7520	218.76	50.701	0.76	-66/+40
Methylamine	1.3634	126.389	102.886	0.32	-70/-10
Water	1.5668	230.298	146.797	0.51	-10/+160
Methanol	1.6807	354.876	48.585	2.05	-98/+50
Ethanol	2.4401	774.414	-15.249	2.66	-98/+70
<i>n</i> -Propanol	2.4907	725.903	37.474	1.10	0/+70
<i>n</i> -Butanol	3.0037	1033.306	-4.3828	0.80	-51/+100
Glycerine	2.8834	997.586	128.481	4.50	-42/+30
Ethylene glycol	1.5923	438.064	141.617	0.18	+20/+100

 $\ln \eta = A + B/(t/^\circ\text{C} + C)$, where t is temperature in $^\circ\text{C}$.

a) Data from Ref. [5].

Table E.6 Dipole moment μ and polarizability volume $\alpha' = \alpha/4\pi\epsilon_0$ for some compounds.^{a)}

Compound	μ (D)	α' (10^{-30} m^3)	Compound	μ (D)	α' (10^{-30} m^3)
He	0	0.201	(CH ₃) ₂ CO	2.84	6.33
Ar	0	1.63	CH ₃ OCH ₃	1.29	5.16
C ₆ H ₆	0	10.3	CH ₃ OH	1.71	3.23
C ₆ H ₅ CH ₃	0.36	–	C ₂ H ₅ OH	1.69	–
C ₆ H ₅ Cl	1.70	12.25	HF	1.91	0.80
CH ₄	0	2.60	HCl	1.03	2.63
CH ₃ Cl	1.86	4.56	HBr	0.79	3.61
CH ₂ Cl ₂	1.58	6.48	HI	0.38	5.45
CHCl ₃	1.02	8.23	N ₂	0	1.76
CCl ₄	0	10.5	O ₂	0	1.60
H ₂ O	1.84	1.49	Cl ₂	0	4.61
NH ₃	1.47	2.26	CO	0.10	1.95
N(CH ₃) ₃	0.60	8.29	CO ₂	0	2.65

a) Dipole moment data from Ref. [6].

Table E.7 Compressibility κ and expansivity α for some solvents at 20 °C.^{a)}

Solvent	ρ (g cm ⁻³)	κ_s (10 ¹¹ Pa ⁻¹)	α_p (10 ³ K ⁻¹)	Solvent	ρ (g cm ⁻³)	κ_s (10 ¹¹ Pa ⁻¹)	α_p (10 ³ K ⁻¹)
<i>n</i> -Hexane	0.654	130	1.36	Water	0.997	45.5	0.257
<i>n</i> -Heptane	0.684	108	–	Methanol	0.792	100	–
<i>n</i> -Octane	0.703	99.3	1.15	Ethanol	0.798	91.1	1.12
Carbon tetrachloride	1.595	71.4	1.22	<i>n</i> -Butyl alcohol	0.810	76.9	–
Benzene	0.878	64.9	1.23	Acetone	0.792	89	–
Toluene	0.866	65.5	1.06	Diethyl ether	0.714	138	1.43
Formamide	1.1292	–	59.1				

a) Data for ρ and κ_s from Ref. [7] (ultrasonic methods determine κ_s , but κ_s can be converted to κ_T using Eq. (2.24)).
Data for α_p from Ref. [8].

Table E.8 Critical data for several organic compounds.^{a)}

Name	Molar mass	ω	T_{cri} (K)	P_{cri} (bar)	V_{cri} (cm ³ mol ⁻¹)	n_{D}	T_{n} (K)
Acetone	58.080	0.307	508.2	47.01	209.	1.3590	329.4
MEK	72.11	0.329	535.6	41.5	267.	1.3788	267
Dimethylether	46.07	0.192	400.0	53.7	178	–	249
Diethylether	74.123	0.281	466.7	36.40	280.	1.353	307.6
Carbon tetrafluoride	88.00	0.191	227.6	37.4	140.	1.0005	145
Carbon tetrachloride	153.822	0.193	556.4	45.60	276.	1.4601	349.8
Chloroform	119.377	0.222	536.4	54.72	239.	1.4459	334.3
Water	18.015	0.345	647.1	220.55	55.9	1.3330	373.2
Methanol	32.042	0.564	512.6	80.97	118.	1.33	337.9
Ethanol	46.069	0.645	513.9	61.48	167.	1.36	351.4
1-Propanol	60.096	0.622	536.8	51.75	219.	1.387	370.4
<i>i</i> -Propanol	60.096	–	508.3	47.6	220	1.3776	356
1-Butanol	74.123	0.594	563.1	44.23	275.	1.399	390.8
Benzene	78.114	0.210	562.2	48.98	259.	–	353.2
Toluene	92.141	0.262	591.8	41.06	316.	1.399	383.8
Ethylbenzene	106.167	0.303	617.2	36.06	374.	–	409.4
Aniline	93.13	0.384	699	53.1	274.	–	457
Pyridine	79.1	0.24	620.0	56.3	254.	1.5093	254
<i>o</i> -Xylene	106.167	0.310	630.3	37.34	369.	1.50545	417.6
<i>m</i> -Xylene	106.167	0.326	617.1	35.36	376.	1.49722	412.3
<i>p</i> -Xylene	106.167	0.322	616.2	35.11	379.	1.49582	411.5
Phenol	94.113	0.444	694.3	61.30	229.	–	455.0
Methane	16.04	0.011	190.6	45.19	98.7	–	111.6
Ethane	30.07	0.100	305.4	48.83	148.	–	184.6
Propane	44.1	0.153	369.85	42.48	200.0	–	231.1
Cyclopropane	42.08	0.264	397.8	54.9	210	–	240
Butane	58.123	0.200	425.1	37.96	255.	–	272.7
Cyclobutane	56.107	0.209	459.9	49.8	210	–	286
Pentane	72.150	0.252	469.7	33.70	313.	1.358	309.2
Cyclopentane	70.134	0.196	511.8	45.02	258.	–	322.4
Neopentane	72.15	0.197	433.8	31.96	311.1	–	282.6
Hexane	86.177	0.301	507.6	30.25	371.	1.375	341.9
Cyclohexane	84.161	0.210	553.6	40.73	308.	1.4262	353.9
Heptane	100.204	0.350	540.2	27.40	428.	1.387	371.6
Octane	114.231	0.400	568.7	24.90	486.	1.398	398.8
Nonane	128.258	0.444	594.6	22.90	544.	1.405	424.0
Acetaldehyde	44.05	0.303	461	56	154	–	293
Acetonitrile	41.05	0.309	508.1	47.0	209	1.344	354
Chlorobenzene	112.56	0.249	632.4	45.2	308	–	404
Trimethylamine	59.11	0.195	433.2	40.7	254	–	270

a) Data from Refs [9] and [10].

MEK, methylethyl ketone.

Table E.9 Physical data for some solvents at 20 °C.^{a)}

Solvent	ϵ	μ (D)	R_M (cm ³)	γ (mN m ⁻²)	ρ (g cm ⁻³)	t_n (°C)
Acetic acid	6.19	1.74	13	26.9	1.0497	117.9
Acetic anhydride	21	2.8	22.4	31.9	1.075	140
Acetone	20.7	2.88	16.2	22.9	0.792	56.3
Acetonitrile	3.44	3.44	0	28.45	0.7768	81.6
Aniline	6.8	1.55	—	42.8	1.022	184.4
Benzene	2.28	0	26.2	28.2	0.878	80.1
Benzyl alcohol	13.1	1.71	32.5	39	1.042	205.2
Bromobenzene	5.4	1.7	34	35.7	1.495	156
Bromoform	4.3	1.3	0	31.7	2.8776	149.6
Butanol	17.5	1.66	0	24.3	1.0269	117.7
<i>i</i> -Butanol	17.7	1.64	22.4	22.5	0.798	107.7
<i>t</i> -Butanol	10.9	1.66	22.2	20	0.7812	82.4
Carbon disulfide	2.6	0	—	31.5	1.2566	46.26
Carbon tetrachloride	2.23	0	26.7	26.2	1.5842	76.8
Chlorobenzene	5.62	1.69	31.1	32.7	1.11	131
Chloroform	4.81	1.04	21.5	26.5	1.4799	61.2
Cyclohexane	2.02	0	27.8	24.4	0.7739	80.7
Dichloromethane	8.93	1.60	16.3	27.3	1.3168	39.8
Diethyl ether	4.34	1.15	22.5	16.5	0.7078	34.6
<i>N,N</i> -Dimethylacetamide	37.8	3.81	24.4	33.3	0.937	165
<i>N,N</i> -Dimethylformamide	36.7	3.86	20	35.2	0.9445	153
Dimethyl sulfoxide	49	3.96	20.1	42.8	1.0958	189
1,4-Dioxane	2.21	0	21.7	32.9	1.0269	101.3
Ethanol	24.3	1.69	14.9	21.8	0.798	78.3
Ethyl acetate	6.02	1.78	22.1	23.2	0.8945	77.1
Ethylene glycol	37.7	2.28	14.5	48.1	1.1097	197.3
Formamide	110	3.7	10.7	58.5	1.1292	210.5
Formic acid	58	1.41	8.6	37.1	1.2131	100.7
Glycerol	42.5	2.56	20.5	62.5	1.2582	290
<i>n</i> -Heptane	1.92	0	34.6	19.8	0.684	98.5
<i>n</i> -Hexane	1.89	0.08	29.9	17.9	0.654	68.7
Methanol	32.6	1.7	8.2	22.4	0.792	64.7
Methyl acetate	6.7	1.72	17.5	24.1	0.932	56.9
<i>n</i> -Methylpyrrolidone	33	4.1	—	—	0.703	202
Nitrobenzene	35	4.22	32.9	42.8	1.1987	210.8
Nitromethane	38.6	3.46	12.5	50.7	1.1312	101.2
<i>n</i> -Pentane	1.84	0	25.3	15.5	0.626	36.2
Propanol	20.1	1.68	17.5	23.4	0.804	97.5
<i>i</i> -Propanol	18.3	1.66	17.6	20.8	0.781	82.3
Pyridine	12.3	2.19	24.1	36.3	0.982	115.3
Tetrahydrofuran	7.32	1.63	19.9	26.9	0.8844	66
Toluene	2.38	0.36	31.1	27.9	0.866	110.6
Water	78.5	1.84	3.7	71.8	0.997	100

a) Data for ϵ , μ , R_M and γ from Ref. [11]. t_n represents the normal boiling point.

Table E.10 Van der Waals constants a and b for several compounds.^{a)}

Compound	a (atm l ² mol ⁻²)	b (10 ⁻² l mol ⁻¹)	Compound	a (atm l ² mol ⁻²)	b (10 ⁻² l mol ⁻¹)
He	0.03457	2.370	C ₆ H ₁₄	24.71	17.35
Ne	0.2135	1.709	H ₂ O	5.536	3.049
Ar	1.363	3.219	H ₂ S	4.490	4.287
Kr	2.349	3.978	CH ₃ OH	9.649	6.702
Xe	4.250	5.105	C ₂ H ₅ OH	12.18	8.407
C ₆ H ₆	18.24	11.54	CH ₃ Cl	7.570	6.483
C ₆ H ₅ CH ₃	24.38	14.63	CCl ₄	19.75	12.81
C ₆ H ₅ F	20.19	12.86	SiCl ₄	4.377	5.786
C ₆ H ₅ Cl	25.77	14.53	(CH ₃) ₂ C=O	14.09	9.94
C ₆ H ₅ Br	28.94	15.39	CO	1.505	3.985
C ₆ H ₅ I	33.52	16.56	CO ₂	3.640	4.267
CH ₄	2.283	4.278	H ₂	0.2476	2.661
C ₂ H ₆	5.562	6.380	O ₂	1.378	3.183
C ₃ H ₈	8.779	8.445	N ₂	1.408	3.913
C ₄ H ₁₀	14.66	12.26	Cl ₂	6.579	5.622
C ₅ H ₁₂	19.26	14.6	NH ₃	4.225	3.707

a) Data from Ref. [12].

Table E.11 Critical data for several inorganic compounds.^{a)}

Name	Molar mass	ω	T_{cri} (K)	P_{cri} (bar)	V_{cri} (cm ³ mol ⁻¹)	Z_{cri}	T_{n} (K)
Ne	20.180	-0.016	44.44	27.605	41.70	0.312	27.1
Ar	39.948	-0.002	150.9	48.98	74.57	0.291	87.3
Kr	83.800	-0.002	209.4	55.00	91.20	0.288	119.7
Xe	131.29	0.002	289.7	58.40	118.0	0.286	165.0
N ₂	28.014	0.037	126.2	33.98	91.10	0.289	77.4
O ₂	31.999	0.022	154.6	50.43	73.4	0.288	90.2
F ₂	37.997	0.051	144.3	52.2	66.2	0.288	85.0
Cl ₂	70.905	0.069	417.2	77.00	124.	0.275	239.1
Br ₂	159.81	0.119	584.1	103.0	135	0.269	331.9
I ₂	253.81	0.229	819	117.0	155.	0.266	457.6
CO	28.01	0.045	132.9	34.94	93.10	0.292	81.7
CO ₂	40.01	0.225	304.1	73.74	94.07	0.247	—
CS ₂	76.14	0.115	552	79.0	170	0.293	319
HF	20.01	0.329	461.0	65.0	69.0	0.117	292.7
HCl	36.46	0.133	324.7	83.1	81.0	0.249	188.2
HBr	80.91	0.069	363.2	85.1	—	—	206.4
HI	127.91	0.038	423.9	90.00	132.7	0.303	237.6
NH ₃	17.031	0.255	405.4	113.53	72.47	0.255	239.8
H ₂ S	34.08	0.090	373.4	89.63	98.00	0.283	212.8

a) Data mainly from Ref. [13].

Table E.12 Antoine constants A , B , and C for the vapor pressure P_{sat} of several compounds.^{a)}

Name	Formula	A	B	C	Range (°C)	$\Delta_{\text{vap}}H_n$ (kJ mol ⁻¹)	t_n (°C)
Acetone	C ₃ H ₆ O	14.3145	2756.22	228.060	-27 to 77	29.10	56.2
MEK	C ₄ H ₈ O	14.1343	2838.4	218.690	-8 to 103	31.30	79.6
Butyl ether	C ₄ H ₁₀ O	14.0735	2511.29	231.200	-43 to 55	26.52	34.4
Carbon tetrachloride	CCl ₄	14.0572	2914.23	232.148	-14 to 101	29.82	76.6
Chloroform	CHCl ₃	13.7324	2548.74	218.552	-23 to 84	29.94	61.1
Dichloromethane	CH ₂ Cl ₂	13.9891	2463.912	223.240	-38 to 60	28.06	39.7
Water	H ₂ O	16.3872	3885.70	230.170	0 to 200	40.66	100.0
Methanol	CH ₄ O	16.5785	3638.27	239.500	-11 to 83	35.21	64.7
Ethanol	C ₂ H ₆ O	16.8958	3795.17	230.918	3 to 96	38.56	78.2
1-Propanol	C ₃ H ₈ O	16.1154	3483.67	205.807	20 to 116	41.44	97.2
2-Propanol	C ₃ H ₈ O	16.6796	3640.20	219.610	8 to 100	39.85	82.2
1-Butanol	C ₄ H ₁₀ O	15.3144	3212.43	182.739	37 to 138	43.29	117.6
2-Butanol	C ₄ H ₁₀ O	15.1989	3026.03	186.500	25 to 120	40.75	99.5
<i>Iso</i> -butanol	C ₄ H ₁₀ O	14.6047	2740.95	166.670	30 to 128	41.82	107.8
<i>Tert</i> -butanol	C ₄ H ₁₀ O	14.8445	2658.29	177.650	10 to 101	39.07	82.3
Benzene	C ₆ H ₆	13.7819	2726.81	217.572	6 to 104	30.73	80.0
Toluene	C ₇ H ₈	13.9320	3056.96	217.625	13 to 136	33.18	110.6
Ethylbenzene	C ₈ H ₁₀	13.9726	3259.93	212.300	33 to 163	35.57	136.2
Phenol	C ₆ H ₆ O	14.4387	3507.80	175.400	20 to 208	46.18	181.8
<i>o</i> -Xylene	C ₈ H ₁₀	14.0415	3358.79	212.041	40 to 172	36.24	144.4
<i>m</i> -Xylene	C ₈ H ₁₀	14.1387	3381.81	216.120	35 to 166	35.66	139.1
<i>p</i> -Xylene	C ₈ H ₁₀	14.0579	3331.45	214.627	35 to 166	35.67	138.3
Phenol	C ₆ H ₆ O	14.4387	3507.80	175.400	80 to 208	46.18	181.8
Butane	C ₄ H ₁₀	13.6608	2154.70	238.789	-73 to 19	22.44	-0.5
<i>Iso</i> -butane	C ₄ H ₁₀	13.8254	2181.79	248.870	-83 to 7	21.30	-11.9
Pentane	C ₅ H ₁₂	13.7667	2451.88	232.014	-45 to 58	25.79	36
Cyclo-pentane	C ₅ H ₁₀	13.9727	2653.90	234.510	-35 to 71	27.30	49.2
Hexane	C ₆ H ₁₄	13.8193	2696.04	224.317	-19 to 92	28.85	68.7
Cyclo-hexane	C ₆ H ₁₂	13.6568	2723.44	220.618	9 to 105	29.97	80.7
Heptane	C ₇ H ₁₆	13.8622	2910.26	216.432	4 to 123	31.77	98.4
Octane	C ₈ H ₁₈	13.9346	3123.13	209.635	26 to 152	43.41	125.6
<i>Iso</i> -octane	C ₈ H ₁₈	13.6703	2896.31	220.767	2 to 125	30.79	99.2
Nonane	C ₉ H ₂₀	13.9854	3311.19	202.694	46 to 178	36.91	150.8
Decane	C ₁₀ H ₂₂	13.9748	3442.76	193.858	65 to 203	38.75	174.1
Acetonitrile	C ₂ H ₃ N	14.8950	3413.10	250.253	-27 to 81	30.19	81.6
Acetic acid	C ₂ H ₄ O ₂	15.0717	3580.80	224.650	24 to 142	23.70	117.9

$\ln P_{\text{sat}}/\text{kPa} = A - B/(t/^\circ\text{C} +)$, where t is the temperature in °C.

$\Delta_{\text{vap}}H_n$ is the enthalpy of evaporation, and t_n the normal boiling temperature.

a) Data from Ref. [9].

MEK, methyl ethyl ketone.

Table E.13 Solubility products K_{sp} of various salts.^{a)}

Compound	K_{sp} at 286 K	Compound	K_{sp} at 286 K	Compound	K_{sp} at 286 K
BaF ₂	1.7×10^{-6}	BaSO ₄	1×10^{-10}	ZnS ^{b)}	1×10^{-23}
CaF ₂	3.4×10^{-11}	SrSO ₄	2.8×10^{-7}	CdS	8×10^{-27}
MgF ₂	6.5×10^{-9}	CaSO ₄	2×10^{-4}	HgS	2×10^{-52}
PbF ₂	3.6×10^{-8}	PbSO ₄	2×10^{-8}	CuS	8.5×10^{-36}
AgCl	1×10^{-10}	AlOH ₃	2×10^{-33}	NiS	2×10^{-21}
CuCl	1.0×10^{-6}	MgOH ₂	1.2×10^{-11}	CoS	8×10^{-22}
HgCl ₂	2.0×10^{-18}	FeOH ₃	1.1×10^{-36}	FeS	3.7×10^{-18}
PbCl ₂	1.7×10^{-5}	FeOH ₂	1.6×10^{-14}	MnS	2.5×10^{-10}
AgI	1.5×10^{-16}	MnOH ₂	4×10^{-14}	Ag ₂ S	1.6×10^{-49}
CuI	5×10^{-12}	NiOH ₂	4×10^{-14}	BaCO ₃	5×10^{-9}
HgI ₂	1.2×10^{-28}	CuOH ₂	1×10^{-19}	CaCO ₃	1×10^{-8}
PbI ₂	1.4×10^{-8}	ZnOH ₂	1.8×10^{-14}	MgCO ₃	2.6×10^{-5}
BaCrO ₄	2.4×10^{-10}	AgOH	1×10^{-8}	PbCO ₃	3.3×10^{-14}
PbCrO ₄	1.8×10^{-14}				
Ag ₂ CrO ₄	1.2×10^{-12}				

a) Data from Ref. [14].

b) Sulfides often crystallize in more than one form, with different solubility products. Values used may differ by as much as 10^9 .**Table E.14** Ionic radii according to Pauling r_p and Shannon-Prewitt r_{sp} for IV and VI coordination.^{a)}

Ion	r_p (pm)	^{IV} r_{sp} (pm)	^{VI} r_{sp} (pm)	Ion	r_p (pm)	^{IV} r_{sp} (pm)	^{VI} r_{sp} (pm)
Li ⁺	60	73	90 (88)	B ³⁺	20	25 (26)	41
Na ⁺	95	113	116	Al ³⁺	50	53	67.5 (67.0)
K ⁺	133	151	152	Sc ³⁺	81	—	88.5 (87.0)
Rb ⁺	148	—	166 (163)	Ga ³⁺	62	61	76
Cs ⁺	169	—	181 (184)	Y ³⁺	93	—	104 (103.2)
Be ²⁺	31	41	59 (45)	In ³⁺	81	76	94 (3)
Mg ²⁺	65	71 (63)	86.0	Fe ³⁺	—	63 HS	69 LS
Ca ²⁺	99	—	114	—	—	—	78.5 HS
Zn ²⁺	74	74	88.0 (88.5)	F ⁻	136	117	119
Sr ²⁺	113	—	132 (130)	Cl ⁻	181	—	167
Ba ²⁺	135	—	149 (150)	Br ⁻	195	—	182
Fe ²⁺	—	77 HS	75 LS	I ⁻	216	—	206
—	—	—	92 HS (91)	O ²⁻	140	124	126
Mn ²⁺	—	80 HS	81 LS	S ²⁻	184	—	170
—	—	—	97 HS (96)	Se ²⁻	198	—	184
Ni ²⁺	—	69	84 (83)	Te ²⁻	221	—	207

a) Data from Refs [15] and [16].

For VI coordination, no brackets indicate the same values reported in 1969 as in 1976; otherwise data in brackets refer to the 1969 report.

LS, low-spin; HS, high-spin.

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