Supplementary File

The Effective Volumes of Waters of Crystallisation: Ionic Systems

Leslie Glasser*

Curtin Institute for Computation, Discipline of Chemistry

Curtin University, GPO Box U1987, Perth, WA 6845, Australia

2 Figures 1 Table ~4 100 words

Supplementary Tables S1-S5

*[a]Corresponding author

L. Glasser: Telephone: + 61 8 9848-3334

E-mail: l.glasser@curtin.edu.au

ORCID iD: 0000-0002-8883-0564

Keywords: hydrate; anhydrate; volume; water of crystallisation; ionic; amino acids

Note: The values of volumes are listed below in nm^3, the basic SI units. They may be converted to $Å^3$, which are secondary SI units, by multiplication by 1 000.

Table S1: Molecular Volumes of Ices and Liquid Water.

Ices and Water	**$\rho(H_2O)$ / g cm^{-3}**	**$V_m(H_2O)^1$ / nm^3**	**$V_m(H_2O)^2$ / nm^3**
Ih Hexagonal	0.93	0.0322	0.0319
Ic Cubic	0.94	0.0318	
III Tetragonal	1.15	0.0260	0.0274
IX Tetragonal	1.16	0.0258	0.0274
II Rhombohedral	1.18	0.0253	0.0254
V Monoclinic	1.24	0.0241	0.0257
IV Rhombohedral	1.27	0.0236	
VI Tetragonal	1.31	0.0228	0.0245
VII Cubic	1.56	0.0192	0.0231
VIII Tetragonal	1.56	0.0192	0.0231
X Cubic	2.51	0.0119	
Liquid H_2O	0.9998	0.0299	0.0300

Table S2: Formula unit molecular volumes, V_m, of hydrates, anhydrates and of waters of crystallisation, $V_m(H_2O)$, of 182 ionic hydrates, *excluding* duplicates from the different sources. Data from Marcus and Jenkins (3:black),[3] Jenkins, Ponikvar-Svet and Liebman (4:green),[4] Mercury (2:gold),[2] "HSC Chemistry 8" (5:blue),[5] Yaws (6:red),[6] updated values from ICSD (7:purple),[7] Li halides (8:purple),[8] and the high hydrates of Mg, Ca and Al halides (9:purple).[9-11] Count = 182; Maximum: 0.0299 nm^3; Mean: 0.023(1) ± 0.004 nm^3; Median: 0.023(5) nm^3; Minimum: 0.0111 nm^3. For the best representative data set, with degrees of hydration two and above: Count = 151; Maximum: 0.0299 nm^3; Mean: 0.024(0) ± 0.003 nm^3; Median: 0.024(2) nm^3; Minimum: 0.0136 nm^3.

Hydrate	V/nm³	$n(H_2O)$	Anhydrate	V/nm³	$V_m(H_2O)$/nm³	Source
$Al_2(SO_4)_3{\cdot}18H_2O$	0.6547	18	$Al_2(SO_4)_3$	0.2096	0.0247	6
$Al_2O_3{\cdot}3H_2O$	0.107	3	Al_2O_3	0.0427	0.0214	5
$Al_2O_3{\cdot}H_2O$	0.0662	1	Al_2O_3	0.0427	0.0235	5
AlBr3·15H2O	0.4793	15	$AlBr_3$	0.1362	0.0229	9
AlBr3·9H2O	0.3607	9	$AlBr_3$	0.1362	0.0249	9
AlCl3·15H2O	0.4550	15	$AlCl_3$	0.0883	0.0244	9
$AlCl_3{\cdot}6H_2O$	0.2402	6	$AlCl_3$	0.0883	0.0253	2
$AlF_3{\cdot}3H_2O$	0.1197	3	AlF_3	0.045	0.0249	5
AlI3·15H2O	0.6160	15	AlI_3	0.1677	0.0299	9
AlI3·17H2O	0.5771	17	AlI_3	0.1677	0.0241	9
$AlI_3{\cdot}6H_2O$	0.3256	6	AlI_3	0.1701	0.0259	6
$Ba(ClO_4)_2{\cdot}3H_2O$	0.2365	3	$Ba(ClO_4)_2$	0.1745	0.0207	6
$Ba(IO_3)_2{\cdot}H_2O$	0.1677	1	$Ba(IO_3)_2$	0.1546	0.0131	6
$Ba(OH)_2{\cdot}8H_2O$	0.2403	8	$Ba(OH)_2$	0.0632	0.0221	5
$BaBr_2{\cdot}2H_2O$	0.1495	2	$BaBr_2$	0.1032	0.0232	6
$BaC_2O_4{\cdot}H_2O$	0.1519	1	BaC_2O_4	0.1408	0.0111	6
$BaCl_2{\cdot}2H_2O$	0.1309	2	$BaCl_2$	0.0886	0.0212	6
$BaCl_2{\cdot}H_2O$	0.1197	1	$BaCl_2$	0.0859	0.0271	2
$BaI_2{\cdot}2H_2O$	0.1657	2	BaI_2	0.126	0.0199	7
$BaN_2O_4{\cdot}H_2O$	0.1291	1	BaN_2O_4	0.1177	0.0114	6
$BeSO_4{\cdot}4H_2O$	0.172	4	$BeSO_4$	0.0698	0.0256	6
$Ca(ClO_4)_2{\cdot}6H_2O$		6			0.0238	3
$Ca(NO_3)_2{\cdot}4H_2O$	0.2154	4	$Ca(NO_3)_2$	0.1088	0.0267	5
$CaBr_2{\cdot}6H_2O$	0.2233	6	$CaBr_2$	0.0935	0.0216	5
CaBr2·9H2O	0.3073	9	$CaBr_2$	0.0982	0.0232	9
$CaC_2O_4{\cdot}2H_2O$	0.1239	2	CaC_2O_4	0.0967	0.0136	5

$CaC_2O_4·H_2O$	0.1103	1	CaC_2O_4	0.0967	0.0136	5
$CaCl_2·2H_2O$	0.1319	2	$CaCl_2$	0.0856	0.0231	6
$CaCl_2·6H_2O$	0.2127	6	$CaCl_2$	0.0856	0.0212	6
$CaHPO_4·2H_2O$	0.1239	2	$CaHPO_4$	0.0774	0.0233	5
CaI2·6.5H2O	0.2859	6.5	CaI_2	0.1210	0.0254	9
$CaI_2·6H_2O$	0.2617	6	CaI_2	0.1232	0.0231	6
CaI2·7H2O	0.2975	7	CaI_2	0.1210	0.0252	9
CaI2·8H2O	0.3262	8	CaI_2	0.1210	0.0256	9
$CaSeO_4·2H_2O$	0.1333	2	$CaSeO_4$	0.078	0.0277	7
$CaSO_4·1/2H_2O$	0.0855	0.5	$CaSO_4$	0.0763	0.0185	2
$CaSO_4·2H_2O$	0.1232	2	$CaSO_4$	0.0764	0.0234	5
$Cd(CH_3COO)_2·2H_2O$	0.2202	2	$Cd(CH_3COO)_2$	0.1635	0.0283	6
$Cd(NO_3)_2·4H_2O$	0.2091	4	$Cd(NO_3)_2$	0.109	0.025	6
$CdCl_2·5/2H_2O$	0.114	2.5	$CdCl_2$	0.0746	0.0157	6
$CdCl_2·H_2O$	0.1038	1	$CdCl_2$	0.0749	0.029	2
$CdSO_4·8/3H_2O$	0.1369	2.67	$CdSO_4$	0.0727	0.0241	2
$CdSO_4·H_2O$	0.0992	1	$CdSO_4$	0.0738	0.0254	5
$CdSO_4·H_2O$	0.0992	1	$CdSO_4$	0.0738	0.0254	6
$Co(NO_3)_2·6H_2O$	0.2584	6	$Co(NO_3)_2$	0.122	0.0227	5
$CoBr_2·6H_2O$	0.2206	6	$CoBr_2$	0.074	0.0244	5
$CoCl_2·2H_2O$	0.1106	2	$CoCl_2$	0.0642	0.0232	2
$CoCl_2·6H_2O$	0.2053	6	$CoCl_2$	0.0642	0.0235	5
$CoF_2·4H_2O$	0.1264	4	CoF_2	0.0361	0.0226	6
$CoI_2·6H_2O$	0.2409	6	CoI_2	0.0927	0.0247	6
$CoSO_4·6H_2O$	0.2184	6	$CoSO_4$	0.0694	0.0248	5
$CoSO_4·7H_2O$	0.2456	7	$CoSO_4$	0.0694	0.0252	5
$CoSO_4·H_2O$	0.0934	1	$CoSO_4$	0.0694	0.024	2
$Cr_2(SO_4)_3·18H_2O$	0.6997	18	$Cr_2(SO_4)_3$	0.21	0.0272	5
$CrPO_4·6H_2O$	0.1997	6	$CrPO_4$	0.053	0.0244	6
$Cu(COOH)_2·4H_2O$	0.207	4	$Cu(COOH)_2$	0.1393	0.0169	6
$CuCl_2·2H_2O$	0.1128	2	$CuCl_2$	0.0659	0.0234	6
$CuF_2·2H_2O$	0.0779	2	CuF_2	0.0399	0.019	6
$CuSO_4·3H_2O$	0.1327	3	$CuSO_4$	0.0679	0.0216	2
$CuSO_4·5H_2O$	0.1813	5	$CuSO_4$	0.0736	0.0215	6
$CuSO_4·H_2O$	0.088	1	$CuSO_4$	0.0679	0.0201	2
$DyCl_3·6H_2O$	0.2445	6	$DyCl_3$	0.1234	0.0202	2
$ErCl_3·6H_2O$	0.2422	6	$ErCl_3$	0.1198	0.0204	2
$EuCl_3·6H_2O$	0.2511	6	$EuCl_3$	0.0877	0.0272	2
$Fe_2(SO_4)_3·9H_2O$	0.4443	9	$Fe_2(SO_4)_3$	0.2142	0.0256	6
$FeBr_2·9H_2O$		9			0.0244	4

$FeCl_2 \cdot 2H_2O$	0.1131	2	$FeCl_2$	0.0666	0.0232	5
$FeCl_2 \cdot 4H_2O$	0.171	4	$FeCl_2$	0.0666	0.0261	5
$FeCl_3 \cdot 6H_2O$	0.2466	6	$FeCl_3$	0.0929	0.0256	6
$FeF_2 \cdot 4H_2O$	0.1252	4	FeF_2	0.0381	0.0218	6
$FeF_3 \cdot 3H_2O$	0.1205	3	FeF_3	0.0484	0.024	6
$FePO_4 \cdot 2H_2O$	0.1141	2		0.0696	0.0223	7
$FePO_4 \cdot 2H_2O$	0.109	2		0.0696	0.0197	7
$FePO_4 \cdot H_2O$	0.087	1		0.0696	0.0174	7
$FeSO_4 \cdot H_2O$	0.095	1	$FeSO_4$	0.0691	0.0259	5
$GdCl_3 \cdot 6H_2O$	0.2546	6	$GdCl_3$	0.0968	0.0263	5
$HoCl_3 \cdot 6H_2O$	0.2425	6	$HoCl_3$	0.1212	0.0202	2
$K_2CO_3 \cdot 3/2H_2O$	0.1343	1.5	K_2CO_3	0.1002	0.0227	6
$K_2CuCl_4 \cdot 2H_2O$	0.2165	2	K_2CuCl_4	0.1755	0.0205	2
$K_3Fe(CN)_6 \cdot 3H_2O$	0.3791	3	$K_3Fe(CN)_6$	0.2892	0.0299	6
$KAl(SO_4)_2 \cdot 12H_2O$	0.4483	12	$KAl(SO_4)_2$	0.1533	0.0246	2
$KF \cdot 2H_2O$	0.0935	2	KF	0.0382	0.0277	7
$KF \cdot 4H_2O$	0.1500	4		0.0382	0.0280	7
$KMgCl_3 \cdot 6H_2O$	0.2865	6	$KMgCl_3$	0.1202	0.0277	2
$KOH \cdot H_2O$		1			0.0171	3
$Li_2SO_4 \cdot H_2O$	0.1031	1	Li_2SO_4	0.0826	0.0205	6
$LiBr \cdot 2H_2O$	0.0885	2	LiBr	0.0415	0.0235	8
$LiBr \cdot 3H_2O$	0.1148	3	LiBr	0.0415	0.0244	8
$LiBr \cdot 5H_2O$	0.1661	5	LiBr	0.0415	0.0249	8
$LiCl \cdot 2H_2O$	0.0791	2	LiCl	0.034	0.0226	8
$LiCl \cdot 3H_2O$	0.1039	3	LiCl	0.034	0.0233	8
$LiCl \cdot 5H_2O$	0.1551	5	LiCl	0.034	0.0242	8
$LiCl \cdot H_2O$	0.0557	1	LiCl	0.034	0.0217	5
$LiClO_4 \cdot 3H_2O$		3			0.0226	3
$LiI \cdot 2H_2O$	0.1056	2	LiI	0.0556	0.0250	8
$LiI \cdot 3H_2O$	0.1316	3	LiI	0.0556	0.0253	8
$LiNO_3 \cdot 3H_2O$		3			0.0273	3
$LiOH \cdot H_2O$	0.0461	1	LiOH	0.0272	0.0189	5
$Mg(ClO_4)_2 \cdot 6H_2O$	0.3056	6	$Mg(ClO_4)_2$	0.1677	0.023	5
$Mg(NO_3)_2 \cdot 2H_2O$	0.2111	2	$Mg(NO_3)_2$	0.1682	0.0214	6
$Mg(NO_3)_2 \cdot 6H_2O$	0.2916	6	$Mg(NO_3)_2$	0.1682	0.0206	6
$MgBr_2 \cdot 6H_2O$	0.2426	6	$MgBr_2$	0.0822	0.0267	6
MgBr2·6H2O	0.2299	6	$MgBr_2$	0.0789	0.0252	9
MgBr2·9H2O	0.3099	9	$MgBr_2$	0.0789	0.0257	9
$MgCl_2 \cdot 12H_2O$		12			0.0291	4
MgCl2·12H2O	0.4166	12	$MgCl_2$	0.0690	0.0290	9
$MgCl_2 \cdot 2H_2O$		2			0.0244	4

$MgCl_2 \cdot 4H_2O$		4			0.0244	4
$MgCl_2 \cdot 6H_2O$	0.2164	6	$MgCl_2$	0.068	0.0247	6
MgCl2·8H2O	0.2734	8	$MgCl_2$	0.0690	0.0256	9
$MgCl_2 \cdot H_2O$		1			0.0242	4
$MgCO_3 \cdot 3H_2O$	0.1242	3	$MgCO_3$	0.0459	0.0261	5
$MgI_2 \cdot 8H_2O$	0.3338	8	MgI_2	0.1042	0.0287	6
MgI2·8H2O	0.3302	8	MgI_2	0.1021	0.0285	9
MgI2·9H2O	0.3421	9	MgI_2	0.1021	0.0267	9
$MgSO_4 \cdot 6H_2O$	0.216	6	$MgSO_4$	0.0751	0.0235	2
$MgSO_4 \cdot 7H_2O$	0.245	7	$MgSO_4$	0.0716	0.0248	6
$MgSO_4 \cdot H_2O$	0.0894	1	$MgSO_4$	0.0716	0.0178	6
$Mn(NO_3)_2 \cdot 6H_2O$		6			0.0207	3
$Mn(NO_3)_2 \cdot 6H_2O$	0.2648	6	$Mn(NO_3)_2$	0.135	0.0216	6
$MnCl_2 \cdot 2H_2O$	0.1175	2	$MnCl_2$	0.0699	0.0238	2
$MnCl_2 \cdot 4H_2O$	0.1718	4	$MnCl_2$	0.0702	0.0254	6
$MnSO_4 \cdot 4H_2O$	0.1639	4	$MnSO_4$	0.0771	0.0217	5
$MnSO_4 \cdot 5H_2O$		5			0.0236	4
$MnSO_4 \cdot 7H_2O$	0.2191	7	$MnSO_4$	0.0771	0.0203	5
$MnSO_4 \cdot H_2O$	0.0951	1	$MnSO_4$	0.0771	0.018	5
$Na(CH_3COO) \cdot 3H_2O$	0.1558	3	$Na(CH_3COO)$	0.0891	0.0222	6
$Na_2B_4O_7 \cdot 10H_2O$	0.366	10	$Na_2B_4O_7$	0.1392	0.0227	6
$Na_2B_4O_7 \cdot 4H_2O$	0.2327	4	$Na_2B_4O_7$	0.1392	0.0234	6
$Na_2B_4O_7 \cdot 5H_2O$	0.2573	5	$Na_2B_4O_7$	0.1392	0.0236	6
$Na_2CO_3 \cdot 10H_2O$	0.3299	10	Na_2CO_3	0.0695	0.026	5
$Na_2CO_3 \cdot 7H_2O$	0.2569	7	Na_2CO_3	0.0695	0.0268	5
$Na_2CO_3 \cdot H_2O$	0.0911	1	Na_2CO_3	0.0695	0.0216	5
$Na_2HPO_4 \cdot 12H_2O$	0.3964	12	Na_2HPO_4	0.1386	0.0215	5
$Na_2HPO_4 \cdot 7H_2O$	0.2618	7	Na_2HPO_4	0.1386	0.0176	5
$Na_2MoO_4 \cdot H_2O$	0.1134	1	Na_2MoO_4	0.0977	0.0157	5
$Na_2S \cdot 9H_2O$	0.2789	9	Na_2S	0.0701	0.0232	6
$Na_2S_2O_3 \cdot 5H_2O$	0.2438	5	$Na_2S_2O_3$	0.1575	0.0173	6
$Na_2SO_3 \cdot 7H_2O$	0.2684	7	Na_2SO_3	0.0796	0.027	6
$Na_2SO_4 \cdot 10H_2O$	0.3664	10	Na_2SO_4	0.0877	0.0279	6
$Na_3PO_4 \cdot 12H_2O$	0.3896	12	Na_3PO_4	0.1073	0.0235	6
$NaBr \cdot 2H_2O$	0.1058	2	NaBr	0.0534	0.0262	6
$NaHSO_4 \cdot H_2O$	0.1092	1	$NaHSO_4$	0.0819	0.0273	6
$NaI \cdot 2H_2O$	0.1261	2	NaI	0.068	0.0291	5
$NaOH \cdot 11/4H_2O$		2.75			0.0235	4
$NaOH \cdot 4H_2O$		4			0.0251	4
$NaOH \cdot 5/2H_2O$		2.5			0.0227	4
$NaOH \cdot 5H_2O$		5			0.0251	4

$NaOH·7/2H_2O$		3.5			0.0235	4
$NaOH·7H_2O$		7			0.025	4
$NaOH·H_2O$		1			0.0238	4
$NdCl_3·6H_2O$	0.2589	6	$NdCl_3$	0.1006	0.0264	5
$NH_4Al(SO_4)_2·12H_2O$	0.4584	12	$NH_4Al(SO_4)_2$	0.159	0.025	2
$NiCl_2·2H_2O$	0.1066	2	$NiCl_2$	0.0606	0.023	5
$NiCl_2·6H_2O$	0.2045	6	$NiCl_2$	0.0609	0.0239	2
$NiSO_4·6H_2O$	0.2102	6	$NiSO_4$	0.0698	0.0234	2
$NiSO_4·7H_2O$	0.2355	7	$NiSO_4$	0.0641	0.0245	6
$NiSO_4·H_2O$	0.0855	1	$NiSO_4$	0.0698	0.0157	2
$Pb(CH_3COO)_2·3H_2O$	0.247	3	$Pb(CH_3COO)_2$	0.1662	0.0269	6
$SmCl_3·6H_2O$	0.2545	6	$SmCl_3$	0.0956	0.0265	6
$SnCl_4·5H_2O$	0.2853	5	$SnCl_4$	0.1632	0.0244	6
$Sr(NO_3)_2·4H_2O$	0.2141	4	$Sr(NO_3)_2$	0.1177	0.0241	5
$SrBr_2·6H_2O$	0.2424	6	$SrBr_2$	0.0962	0.0244	7
$SrBr_2·H_2O$	0.1136	1	$SrBr_2$	0.0962	0.0174	7
$SrCl_2·2H_2O$	0.1209	2	$SrCl_2$	0.0862	0.0173	2
$SrCl_2·6H_2O$	0.2258	6	$SrCl_2$	0.0862	0.0233	6
$SrCl_2·H_2O$	0.1004	1	$SrCl_2$ 3	0.0854	0.015	2
$SrI_2·2H_2O$		2			0.0232	4
$SrI_2·6H_2O$		6			0.0241	4
$SrI_2·H_2O$		1			0.0219	4
$UO_2Cl_2·3H_2O$	0.1853	3	UO_2Cl_2	0.1049	0.0268	2
$UO_2SO_4·3H_2O$	0.1799	3	UO_2SO_4	0.1206	0.0197	2
$UO_2SO_4·5/2H_2O$	0.1912	2.5	UO_2SO_4 4	0.1206	0.0282	2
$UO_2SO_4·7/2H_2O$	0.2019	3.5	UO_2SO_4	0.1206	0.0232	2
$YbCl_3·6H_2O$	0.2499	6	$YbCl_3$	0.0935	0.0261	5
$ZnSO_4·6H_2O$	0.216	6	$ZnSO_4$	0.0705	0.0242	5
$ZnSO_4·7H_2O$	0.244	7	$ZnSO_4$	0.0705	0.0248	5
$ZnSO_4·H_2O$	0.0931	1	$ZnSO_4$	0.0705	0.0226	5
$Zr(SO_4)_2·4H_2O$	0.2107	4	$Zr(SO_4)_2$	0.1461	0.0162	6
$Zr(SO_4)_2·5H_2O$	0.2427	5	$Zr(SO_4)_2$	0.1276	0.0230	7
$Zr(SO_4)_2·5H_2O$	0.2535	5	$Zr(SO_4)_2$	0.1276	0.0252	7
$Zr(SO_4)_2·7H_2O$	0.3146	7	$Zr(SO_4)_2$	0.1276	0.0267	7

Table S3: Formula unit molecular volumes, V_m, of hydrates, anhydrates and of waters of crystallisation, $V_m(H_2O)$, of 300 inorganic hydrates, *including* duplicates from the different sources and outliers. Unedited data from Marcus and Jenkins (3:black),[3] Jenkins, Ponikvar-Svet and Liebman (4:green),[4] Mercury (2:gold),[2] "HSC Chemistry 8" (5:blue),[5] and Yaws (6:red).[6] Maximum: 0.0351 nm^3; Mean: 0.022(6) ± 0.004 nm^3; Minimum: 0.0070 nm^3 (the statistical data includes both duplicates and outliers).

Hydrate	V_m/nm³	$n(H_2O)$	Anhydrate	V_m/nm³	$V_m(H_2O)$/nm³	Source
$Al_2(SO_4)_3{\cdot}18H_2O$	0.6547	18	$Al_2(SO_4)_3$	0.2096	0.0247	6
$Al_2O_3{\cdot}H_2O$	0.0662	1	Al_2O_3	0.0427	0.0235	5
$Al_2O_3{\cdot}3H_2O$	0.1070	3	Al_2O_3	0.0427	0.0214	5
$AlBr_3{\cdot}6H_2O$	0.2450	6	$AlBr_3$	0.1384	0.0178	6
$AlCl_3{\cdot}6H_2O$	0.2402	6	$AlCl_3$	0.0883	0.0253	2
$AlCl_3{\cdot}6H_2O$	0.1672	6	$AlCl_3$	0.0893	0.0130	5
$AlF_3{\cdot}3H_2O$	0.1197	3	AlF_3	0.0450	0.0249	5
$AlF_3{\cdot}3H_2O$	0.1197	3	AlF_3	0.0450	0.0249	6
$AlI_3{\cdot}6H_2O$	0.3256	6	AlI_3	0.1701	0.0259	6
$Ba(ClO_4)_2{\cdot}3H_2O$	0.2365	3	$Ba(ClO_4)_2$	0.1745	0.0207	5
$Ba(ClO_4)_2{\cdot}3H_2O$	0.2365	3	$Ba(ClO_4)_2$	0.1745	0.0207	6
$Ba(IO_3)_2{\cdot}H_2O$	0.1677	1	$Ba(IO_3)_2$	0.1546	0.0131	6
$Ba(OH)_2{\cdot}8H_2O$	0.2403	8	$Ba(OH)_2$	0.0632	0.0221	5
$BaBr_2{\cdot}2H_2O$		2			0.0204	3
$BaBr_2{\cdot}2H_2O$	0.1545	2	$BaBr_2$	0.1032	0.0257	5
$BaBr_2{\cdot}2H_2O$	0.1495	2	$BaBr_2$	0.1032	0.0232	6
$BaC_2O_4{\cdot}H_2O$	0.1519	1	BaC_2O_4	0.1408	0.0111	6
$BaCl_2{\cdot}H_2O$	0.1130	1	$BaCl_2$	0.0859	0.0271	2
$BaCl_2{\cdot}H_2O$	0.1197	1	$BaCl_2$	0.0859	0.0271	2
$BaCl_2{\cdot}2H_2O$		2			0.0212	4
$BaCl_2{\cdot}2H_2O$	0.1359	2	$BaCl_2$	0.0859	0.0250	2
$BaCl_2{\cdot}2H_2O$	0.1359	2	$BaCl_2$	0.0859	0.0250	2
$BaCl_2{\cdot}2H_2O$	0.1308	2	$BaCl_2$	0.0886	0.0211	5
$BaCl_2{\cdot}2H_2O$	0.1309	2	$BaCl_2$	0.0886	0.0212	6
$BaI_2{\cdot}2H_2O$	0.1377	2	BaI_2	0.1261	0.0091	5
$BaI_2{\cdot}2H_2O$	0.1418	2	BaI_2	0.1261	0.0079	6
$BaN_2O_4{\cdot}H_2O$	0.1291	1	BaN_2O_4	0.1177	0.0114	6
$BeSO_4{\cdot}4H_2O$	0.1720	4	$BeSO_4$	0.0715	0.0251	5
$BeSO_4{\cdot}4H_2O$	0.1720	4	$BeSO_4$	0.0698	0.0256	6
$Ca(ClO_4)_2{\cdot}6H_2O$		6			0.0238	3

$Ca(NO_3)_2{\cdot}4H_2O$		4			0.0242	3
$Ca(NO_3)_2{\cdot}4H_2O$	0.2154	4	$Ca(NO_3)_2$	0.1088	0.0267	5
$CaBr_2{\cdot}6H_2O$		6			0.0231	3
$CaBr_2{\cdot}6H_2O$	0.2233	6	$CaBr_2$	0.0935	0.0216	5
$CaC_2O_4{\cdot}H_2O$		1			0.0123	4
$CaC_2O_4{\cdot}H_2O$	0.1103	1	CaC_2O_4	0.0967	0.0136	5
$CaC_2O_4{\cdot}H_2O$	0.1103	1	CaC_2O_4	0.0967	0.0136	6
$CaC_2O_4{\cdot}2H_2O$	0.1239	2	CaC_2O_4	0.0967	0.0136	5
$CaCl_2{\cdot}2H_2O$	0.1319	2	$CaCl_2$	0.0856	0.0231	6
$CaCl_2{\cdot}6H_2O$	0.2127	6	$CaCl_2$	0.0857	0.0212	5
$CaCl_2{\cdot}6H_2O$	0.2127	6	$CaCl_2$	0.0856	0.0212	6
$CaHPO_4{\cdot}2H_2O$		2			0.0228	4
$CaHPO_4{\cdot}2H_2O$	0.1239	2	$CaHPO_4$	0.0774	0.0233	5
$CaI_2{\cdot}6H_2O$	0.2617	6	CaI_2	0.1232	0.0231	6
$CaSeO_4{\cdot}2H_2O$	0.1323	2	$CaSeO_4$	0.1055	0.0134	5
$CaSO_4{\cdot}1/2H_2O$		0.5			0.0183	4
$CaSO_4{\cdot}1/2H_2O$	0.0869	0.5	$CaSO_4$	0.0763	0.0211	2
$CaSO_4{\cdot}1/2H_2O$ 3	0.0838	0.5	$CaSO_4$	0.0753	0.0170	2
$CaSO_4{\cdot}1/2H_2O$ 4	0.0855	0.5	$CaSO_4$	0.0763	0.0185	2
$CaSO_4{\cdot}2H_2O$		2			0.0233	4
$CaSO_4{\cdot}2H_2O$	0.1234	2	$CaSO_4$	0.0763	0.0236	2
$CaSO_4{\cdot}2H_2O$	0.1240	2	$CaSO_4$	0.0763	0.0239	2
$CaSO_4{\cdot}2H_2O$	0.1230	2	$CaSO_4$	0.0763	0.0234	2
$CaSO_4{\cdot}2H_2O$	0.1240	2	$CaSO_4$	0.0763	0.0239	2
$CaSO_4{\cdot}2H_2O$	0.1232	2	$CaSO_4$	0.0764	0.0234	5
$Cd(CH_3COO)_2{\cdot}2H_2O$	0.2202	2	$Cd(CH_3COO)_2$	0.1635	0.0283	6
$Cd(NO_3)_2{\cdot}4H_2O$		4			0.0246	3
$Cd(NO_3)_2{\cdot}4H_2O$	0.2082	4	$Cd(NO_3)_2$	0.1090	0.0248	5
$Cd(NO_3)_2{\cdot}4H_2O$	0.2091	4	$Cd(NO_3)_2$	0.1090	0.0250	6
$CdCl_2{\cdot}H_2O$	0.1038	1	$CdCl_2$	0.0749	0.0290	2
$CdCl_2{\cdot}5/2H_2O$	0.1376	2.5	$CdCl_2$	0.0749	0.0251	2
$CdCl_2{\cdot}5/2H_2O$	0.1140	2.5	$CdCl_2$	0.0746	0.0157	5
$CdCl_2{\cdot}5/2H_2O$	0.1140	2.5	$CdCl_2$	0.0746	0.0157	6
$CdSO_4{\cdot}H_2O$	0.0995	1	$CdSO_5$	0.0727	0.0268	2
$CdSO_4{\cdot}H_2O$	0.0992	1	$CdSO_4$	0.0738	0.0254	5
$CdSO_4{\cdot}H_2O$	0.0992	1	$CdSO_4$	0.0738	0.0254	6
$CdSO_4{\cdot}8/3H_2O$	0.1379	2.67	$CdSO_4$	0.0738	0.0240	5
$CdSO_4{\cdot}8/3H_2O$	0.1369	2.67	$CdSO_4$	0.0727	0.0241	2
$Co(NO_3)_2{\cdot}6H_2O$		6			0.0208	3
$Co(NO_3)_2{\cdot}6H_2O$		6			0.0223	4
$Co(NO_3)_2{\cdot}6H_2O$	0.2584	6	$Co(NO_3)_2$	0.1220	0.0227	5
$CoBr_2{\cdot}6H_2O$		6			0.0250	3
$CoBr_2{\cdot}6H_2O$	0.2206	6	$CoBr_2$	0.0740	0.0244	5
$CoCl_2{\cdot}2H_2O$	0.1090	2	$CoCl_2$	0.0625	0.0233	2

$CoCl_2 \cdot 2H_2O$	0.1106	2	$CoCl_2$	0.0642	0.0232	2
$CoCl_2 \cdot 2H_2O$	0.1112	2	$CoCl_2$	0.0642	0.0235	6
$CoCl_2 \cdot 6H_2O$	0.2057	6	$CoCl_2$	0.0642	0.0236	2
$CoCl_2 \cdot 6H_2O$	0.2053	6	$CoSO_4$	0.0684	0.0228	2
$CoCl_2 \cdot 6H_2O$	0.2053	6	$CoCl_2$	0.0642	0.0235	5
$CoCl_2 \cdot 6H_2O$	0.2053	6	$CoCl_2$	0.0642	0.0235	6
$CoF_2 \cdot 4H_2O$	0.1264	4	CoF_2	0.0361	0.0226	6
$CoI_2 \cdot 6H_2O$	0.2409	6	CoI_2	0.0927	0.0247	6
$CoSO_4 \cdot H_2O$		1			0.0236	4
$CoSO_4 \cdot H_2O$	0.0883	1	$CoSO_4$	0.0667	0.0216	2
$CoSO_4 \cdot H_2O$	0.0934	1	$CoSO_4$	0.0694	0.0240	2
$CoSO_4 \cdot H_2O$	0.0933	1	$CoSO_4$	0.0694	0.0239	6
$CoSO_4 \cdot 6H_2O$		6			0.0244	4
$CoSO_4 \cdot 6H_2O$	0.2163	6	$CoSO_4$	0.0694	0.0245	2
$CoSO_4 \cdot 6H_2O$	0.2184	6	$CoSO_4$	0.0694	0.0248	5
$CoSO_4 \cdot 7H_2O$		7			0.0252	4
$CoSO_4 \cdot 7H_2O$	0.2448	7	$CoSO_4$ (sol-3)	0.0694	0.0251	2
$CoSO_4 \cdot 7H_2O$	0.2396	7	$CoSO_4$	0.0694	0.0243	2
$CoSO_4 \cdot 7H_2O$	0.2456	7	$CoSO_4$	0.0694	0.0252	5
$CoSO_4 \cdot 7H_2O$	0.2299	7	$CoSO_4$	0.0694	0.0229	6
$Cr_2(SO_4)_3 \cdot 18H_2O$		18			0.0244	4
$Cr_2(SO_4)_3 \cdot 18H_2O$	0.6997	18	$Cr_2(SO_4)_3$	0.2100	0.0272	5
$CrPO_4 \cdot 6H_2O$	0.1997	6	$CrPO_4$	0.0530	0.0244	6
$Cu(COOH)_2 \cdot 4H_2O$	0.2070	4	$Cu(COOH)_2$	0.1393	0.0169	6
$CuCl_2 \cdot 2H_2O$	0.1104	2	$CuCl_2$	0.0649	0.0227	2
$CuCl_2 \cdot 2H_2O$	0.1128	2	$CuCl_2$	0.0659	0.0234	5
$CuCl_2 \cdot 2H_2O$	0.1128	2	$CuCl_2$	0.0659	0.0234	6
$CuF_2 \cdot 2H_2O$	0.0779	2	CuF_2	0.0399	0.0190	5
$CuF_2 \cdot 2H_2O$	0.0779	2	CuF_2	0.0399	0.0190	6
$CuSO_4 \cdot H_2O$		1			0.0111	4
$CuSO_4 \cdot H_2O$	0.0880	1	$CuSO_4$	0.0679	0.0201	2
$CuSO_4 \cdot 3H_2O$		3			0.0198	4
$CuSO_4 \cdot 3H_2O$	0.1327	3	$CuSO_4$	0.0679	0.0216	2
$CuSO_4 \cdot 5H_2O$		5			0.0217	4
$CuSO_4 \cdot 5H_2O$	0.1811	5	$CuSO_4$	0.0679	0.0226	2
$CuSO_4 \cdot 5H_2O$	0.1809	5	$CuSO_4$	0.0679	0.0226	2
$CuSO_4 \cdot 5H_2O$	0.1815	5	$CuSO_4$	0.0679	0.0227	2
$CuSO_4 \cdot 5H_2O$	0.1809	5	$CuSO_4$	0.0679	0.0226	2
$CuSO_4 \cdot 5H_2O$	0.1813	5	$CuSO_4$	0.0735	0.0216	5
$CuSO_4 \cdot 5H_2O$	0.1813	5	$CuSO_4$	0.0736	0.0215	6
$DyCl_3 \cdot 6H_2O$	0.2445	6	$DyCl_3$	0.1234	0.0202	2
$ErCl_3 \cdot 6H_2O$	0.2422	6	$ErCl_3$	0.1198	0.0204	2

$EuCl_3 \cdot 6H_2O$	0.2511	6	$EuCl_3$	0.0877	0.0272	2
$Fe_2(SO_4)_3 \cdot 9H_2O$	0.4443	9	$Fe_2(SO_4)_3$	0.2142	0.0256	6
$FeBr_2 \cdot 9H_2O$		9			0.0244	4
$FeCl_2 \cdot 2H_2O$	0.1131	2	$FeCl_2$	0.0666	0.0232	5
$FeCl_2 \cdot 2H_2O$	0.1131	2	$FeCl_2$	0.0705	0.0213	6
$FeCl_2 \cdot 4H_2O$	0.1710	4	$FeCl_2$	0.0666	0.0261	5
$FeCl_2 \cdot 4H_2O$	0.1710	4	$FeCl_2$	0.0705	0.0251	6
$FeCl_3 \cdot 6H_2O$		6			0.0257	3
$FeCl_3 \cdot 6H_2O$	0.2466	6	$FeCl_3$	0.0929	0.0256	6
$FeF_2 \cdot 4H_2O$	0.1252	4	FeF_2	0.0381	0.0218	6
$FeF_3 \cdot 3H_2O$	0.1205	3	FeF_3	0.0484	0.0240	6
$FePO_4 \cdot 2H_2O$		2			0.0150	4
$FeSO_4 \cdot H_2O$	0.0909	1	$FeSO_4$	0.0690	0.0219	2
$FeSO_4 \cdot H_2O$	0.0950	1	$FeSO_4$	0.0691	0.0259	5
$FeSO_4 \cdot H_2O$	0.0940	1	$FeSO_4$	0.0691	0.0249	6
$FeSO_4 \cdot 7H_2O$		7			0.0248	4
$FeSO_4 \cdot 7H_2O$	0.2416	7	$FeSO_4$	0.0690	0.0247	2
$FeSO_4 \cdot 7H_2O$	0.2432	7	$FeSO_4$	0.0690	0.0249	2
$FeSO_4 \cdot 7H_2O$	0.2429	7	$FeSO_4$	0.0691	0.0248	5
$FeSO_4 \cdot 7H_2O$	0.2436	7	$FeSO_4$	0.0691	0.0249	6
$GdCl_3 \cdot 6H_2O$	0.2546	6	$GdCl_3$	0.0968	0.0263	5
$Hg(NO_3)_2 \cdot H_2O$	0.1323	1	$Hg(NO_3)_2$	0.1253	0.0070	6
$HoCl_3 \cdot 6H_2O$	0.2425	6	$HoCl_3$	0.1212	0.0202	2
$K_2CO_3 \cdot 3/2H_2O$	0.1343	1.5	K_2CO_3	0.1002	0.0227	6
$K_2CuCl_4 \cdot 2H_2O$	0.2165	2	K_2CuCl_4	0.1755	0.0205	2
$K_3Fe(CN)_6 \cdot 3H_2O$	0.3791	3	$K_3Fe(CN)_6$	0.2892	0.0299	6
$K_4Fe(CN)_6 \cdot 3H_2O$		3			0.0121	4
$KAl(SO_4)_2 \cdot 12H_2O$	0.4493	12	$KAl(SO_4)_2$	0.1527	0.0247	2
$KAl(SO_4)_2 \cdot 12H_2O$	0.4483	12	$KAl(SO_4)_2$	0.1533	0.0246	2
$KF \cdot 2H_2O$		2			0.0269	4
$KF \cdot 2H_2O$	0.0625	2	KF	0.0389	0.0118	5
$KF \cdot 2H_2O$	0.0625	2	KF	0.0389	0.0118	6
$KF \cdot 4H_2O$		4			0.0278	4
$KMgCl_3 \cdot 6H_2O$	0.2865	6	$KMgCl_3$	0.1202	0.0277	2
$KOH \cdot H_2O$		1			0.0171	3
$La_2(SO_4)_3 \cdot 9H_2O$		9			0.0181	4
$La_2(SO_4)_3 \cdot 9H_2O$	0.4287	9	$La_2(SO_4)_3$	0.2610	0.0186	5
$Li_2SO_4 \cdot H_2O$		1			0.0192	4
$Li_2SO_4 \cdot H_2O$	0.1039	1	Li_2SO_4	0.0825	0.0214	2
$Li_2SO_4 \cdot H_2O$	0.1031	1	Li_2SO_4	0.0826	0.0205	5
$Li_2SO_4 \cdot H_2O$	0.1031	1	Li_2SO_4	0.0826	0.0205	6
$LiCl \cdot H_2O$	0.0569	1	LiCl	0.0342	0.0227	2

$LiCl \cdot H_2O$	0.0557	1	LiCl	0.0340	0.0217	5
$LiClO_4 \cdot 3H_2O$		3			0.0226	3
$LiI \cdot 2H_2O$		2			0.0254	3
$LiI \cdot 3H_2O$	0.0891	3	LiI	0.0547	0.0115	5
$LiI \cdot 3H_2O$	0.0896	3	LiI	0.0545	0.0117	6
$LiNO_3 \cdot 3H_2O$		3			0.0273	3
$LiOH \cdot H_2O$	0.0461	1	LiOH	0.0272	0.0189	5
$Mg(ClO_4)_2 \cdot 6H_2O$		6			0.0181	3
$Mg(ClO_4)_2 \cdot 6H_2O$	0.3056	6	$Mg(ClO_4)_2$	0.1677	0.0230	5
$Mg(NO_3)_2 \cdot 2H_2O$	0.2111	2	$Mg(NO_3)_2$	0.1682	0.0214	6
$Mg(NO_3)_2 \cdot 6H_2O$		6			0.0254	3
$Mg(NO_3)_2 \cdot 6H_2O$	0.2596	6	$Mg(NO_3)_2$	0.1071	0.0254	5
$Mg(NO_3)_2 \cdot 6H_2O$	0.2916	6	$Mg(NO_3)_2$	0.1682	0.0206	6
$MgBr_2 \cdot 6H_2O$		6			0.0253	3
$MgBr_2 \cdot 6H_2O$	0.2426	6	$MgBr_2$	0.0822	0.0267	5
$MgBr_2 \cdot 6H_2O$	0.2426	6	$MgBr_2$	0.0822	0.0267	6
$MgCl_2 \cdot 12H_2O$		12			0.0291	4
$MgCl_2 \cdot H_2O$		1			0.0242	4
$MgCl_2 \cdot 2H_2O$		2			0.0244	4
$MgCl_2 \cdot 4H_2O$		4			0.0244	4
$MgCl_2 \cdot 6H_2O$		6			0.0240	3
$MgCl_2 \cdot 6H_2O$		6			0.0245	4
$MgCl_2 \cdot 6H_2O$	0.2151	6	$MgCl_2$	0.0680	0.0245	5
$MgCl_2 \cdot 6H_2O$	0.2164	6	$MgCl_2$	0.0680	0.0247	6
$MgCO_3 \cdot 3H_2O$	0.1242	3	$MgCO_3$	0.0459	0.0261	5
$MgI_2 \cdot 8H_2O$	0.3338	8	MgI_2	0.1042	0.0287	6
$MgSO_4 \cdot H_2O$	0.0894	1	$MgSO_4$	0.0751	0.0143	5
$MgSO_4 \cdot H_2O$	0.0894	1	$MgSO_4$	0.0716	0.0178	6
$MgSO_4 \cdot 6H_2O$		6			0.0241	4
$MgSO_4 \cdot 6H_2O$	0.2160	6	$MgSO_4$	0.0751	0.0235	2
$MgSO_4 \cdot 7H_2O$	0.2438	7	$MgSO_4$	0.0751	0.0241	2
$MgSO_4 \cdot 7H_2O$	0.2436	7	$MgSO_4$	0.0751	0.0241	5
$MgSO_4 \cdot 7H_2O$	0.2450	7	$MgSO_4$	0.0716	0.0248	6
$Mn(NO_3)_2 \cdot 4H_2O$	0.1957	4	$Mn(NO_3)_2$	0.1350	0.0152	6
$Mn(NO_3)_2 \cdot 6H_2O$		6			0.0207	3
$Mn(NO_3)_2 \cdot 6H_2O$	0.2648	6	$Mn(NO_3)_2$	0.1350	0.0216	6
$MnCl_2 \cdot 2H_2O$	0.1175	2	$MnCl_2$	0.0699	0.0238	2
$MnCl_2 \cdot 4H_2O$		4			0.0230	3
$MnCl_2 \cdot 4H_2O$	0.1636	4	$MnCl_2$	0.0699	0.0234	2
$MnCl_2 \cdot 4H_2O$	0.1718	4	$MnCl_2$	0.0702	0.0254	5
$MnCl_2 \cdot 4H_2O$	0.1718	4	$MnCl_2$	0.0702	0.0254	6
$MnSO_4 \cdot H_2O$	0.0951	1	$MnSO_4$	0.0771	0.0180	5
$MnSO_4 \cdot 4H_2O$	0.1639	4	$MnSO_4$	0.0771	0.0217	5

$MnSO_4 \cdot 5H_2O$		5			0.0236	4
$MnSO_4 \cdot 7H_2O$	0.2191	7	$MnSO_4$	0.0771	0.0203	5
$Na(CH_3COO) \cdot 3H_2O$	0.1558	3	$Na(CH_3COO)$	0.0891	0.0222	6
$Na_2B_4O_7 \cdot 10H_2O$		10			0.0267	4
$Na_2B_4O_7 \cdot 10H_2O$	0.3660	10	$Na_2B_4O_7$	0.1411	0.0225	5
$Na_2B_4O_7 \cdot 10H_2O$	0.3660	10	$Na_2B_4O_7$	0.1392	0.0227	6
$Na_2B_4O_7 \cdot 4H_2O$	0.2327	4	$Na_2B_4O_7$	0.1392	0.0234	6
$Na_2B_4O_7 \cdot 5H_2O$	0.2573	5	$Na_2B_4O_7$	0.1392	0.0236	6
$Na_2CO_3 \cdot 10H_2O$		10			0.0252	4
$Na_2CO_3 \cdot 10H_2O$	0.3299	10	Na_2CO_3	0.0695	0.0260	5
$Na_2CO_3 \cdot 10H_2O$	0.3254	10	Na_2CO_3	0.0693	0.0256	6
$Na_2CO_3 \cdot H_2O$		1			0.0311	4
$Na_2CO_3 \cdot H_2O$	0.0911	1	Na_2CO_3	0.0695	0.0216	5
$Na_2CO_3 \cdot H_2O$	0.0915	1	Na_2CO_3	0.0693	0.0222	6
$Na_2CO_3 \cdot 7H_2O$	0.2569	7	Na_2CO_3	0.0695	0.0268	5
$Na_2HPO_4 \cdot 12H_2O$	0.3964	12	Na_2HPO_4	0.1386	0.0215	5
$Na_2HPO_4 \cdot 7H_2O$	0.2618	7	Na_2HPO_4	0.1386	0.0176	5
$Na_2MoO_4 \cdot H_2O$	0.1134	1	Na_2MoO_4	0.0977	0.0157	5
$Na_2S \cdot 5H_2O$	0.1767	5	Na_2S	0.0701	0.0213	6
$Na_2S \cdot 9H_2O$	0.2789	9	Na_2S	0.0701	0.0232	6
$Na_2S_2O_3 \cdot 5H_2O$	0.2438	5	$Na_2S_2O_3$	0.1575	0.0173	5
$Na_2S_2O_3 \cdot 5H_2O$	0.2438	5	$Na_2S_2O_3$	0.1575	0.0173	6
$Na_2SO_3 \cdot 7H_2O$	0.2684	7	Na_2SO_3	0.0796	0.0270	6
$Na_2SO_4 \cdot 10H_2O$		10			0.0277	4
$Na_2SO_4 \cdot 10H_2O$	0.3650	10	Na_2SO_4 3	0.0886	0.0276	2
$Na_2SO_4 \cdot 10H_2O$	0.3649	10	Na_2SO_4	0.0886	0.0276	2
$Na_2SO_4 \cdot 10H_2O$	0.3629	10	Na_2SO_4	0.0885	0.0274	2
$Na_2SO_4 \cdot 10H_2O$	0.3649	10	Na_2SO_4 [O]	0.0876	0.0277	2
$Na_2SO_4 \cdot 10H_2O$	0.3654	10	Na_2SO_4	0.0880	0.0277	5
$Na_2SO_4 \cdot 10H_2O$	0.3664	10	Na_2SO_4	0.0877	0.0279	6
$Na_3PO_4 \cdot 12H_2O$	0.3896	12	Na_3PO_4	0.1073	0.0235	6
$NaBr \cdot 2H_2O$	0.1058	2	NaBr	0.0533	0.0262	5
$NaBr \cdot 2H_2O$	0.1058	2	NaBr	0.0534	0.0262	6
$NaHSO_4 \cdot H_2O$	0.1088	1	$NaHSO_4$	0.0834	0.0254	2
$NaHSO_4 \cdot H_2O$	0.1092	1	$NaHSO_4$	0.0819	0.0273	6
$NaI \cdot 2H_2O$	0.1261	2	NaI	0.0680	0.0291	5
$NaIO_4 \cdot 3H_2O$	0.1382	3	$NaIO_4$	0.0920	0.0154	6
$NaOH \cdot H_2O$		1			0.0245	3
$NaOH \cdot H_2O$		1			0.0238	4
$NaOH \cdot 5/2H_2O$		2.5			0.0227	4
$NaOH \cdot 11/4H_2O$		2.75			0.0235	4

$NaOH·7/2H_2O$		3.5			0.0235	4
$NaOH·4H_2O$		4			0.0251	4
$NaOH·5H_2O$		5			0.0251	4
$NaOH·7H_2O$		7			0.0250	4
$NdCl_3·6H_2O$	0.2589	6	$NdCl_3$	0.1006	0.0264	5
$NH_4Al(SO_4)_2·12H_2O$	0.4584	12	$NH_4Al(SO_4)_2$	0.1590	0.0250	2
$NiCl_2·2H_2O$	0.1064	2	$NiCl_2$	0.0622	0.0221	2
$NiCl_2·2H_2O$	0.1064	2	$NiCl_2$	0.0609	0.0227	2
$NiCl_2·2H_2O$	0.1066	2	$NiCl_2$	0.0606	0.0230	5
$NiCl_2·6H_2O$		6			0.0233	3
$NiCl_2·6H_2O$	0.2045	6	$NiCl_2$	0.0609	0.0239	2
$NiSO_4·H_2O$	0.0855	1	$NiSO_4$	0.0698	0.0157	2
$NiSO_4·6H_2O$		6			0.0242	4
$NiSO_4·6H_2O$	0.2098	6	$NiSO_4$	0.0641	0.0243	2
$NiSO_4·6H_2O$	0.2108	6	$NiSO_4$	0.0641	0.0245	5
$NiSO_4·6H_2O$	0.2108	6	$NiSO_4$	0.0641	0.0245	6
$NiSO_4·6H_2O$	0.2102	6	$NiSO_4$	0.0698	0.0234	2
$NiSO_4·6H_2O$	0.2102	6	$NiSO_4$	0.0698	0.0234	2
$NiSO_4·7H_2O$		7			0.0257	4
$NiSO_4·7H_2O$	0.2439	7	$NiSO_4$	0.0641	0.0257	2
$NiSO_4·7H_2O$	0.2388	7	$NiSO_4$	0.0698	0.0241	2
$NiSO_4·7H_2O$	0.2394	7	$NiSO_4$	0.0698	0.0242	2
$NiSO_4·7H_2O$	0.2355	7	$NiSO_4$	0.0641	0.0245	5
$NiSO_4·7H_2O$	0.2355	7	$NiSO_4$	0.0641	0.0245	6
$Pb(CH_3COO)_2·3H_2O$	0.2470	3	$Pb(CH_3COO)_2$	0.1662	0.0269	6
$SmCl_3·6H_2O$	0.2545	6	$SmCl_3$	0.0956	0.0265	5
$SmCl_3·6H_2O$	0.2545	6	$SmCl_3$	0.0956	0.0265	6
$SnCl_4·5H_2O$	0.2853	5	$SnCl_4$	0.1632	0.0244	6
$Sr(NO_3)_2·4H_2O$	0.2141	4	$Sr(NO_3)_2$	0.1177	0.0241	5
$SrBr_2·H_2O$		1			0.0136	4
$SrBr_2·6H_2O$		6			0.0241	4
$SrBr_2·6H_2O$	0.2470	6	$SrBr_2$	0.0974	0.0249	5
$SrBr_2·6H_2O$	0.2474	6	$SrBr_2$	0.0974	0.0250	6
$SrCl_2·H_2O$		1			0.0351	4
$SrCl_2·H_2O$	0.1004	1	$SrCl_2$ 3	0.0854	0.0150	2
$SrCl_2·2H_2O$		2			0.0164	4
$SrCl_2·2H_2O$	0.1194	2	$SrCl_2$	0.0862	0.0166	2
$SrCl_2·2H_2O$	0.1209	2	$SrCl_2$	0.0862	0.0173	2

$SrCl_2 \cdot 6H_2O$	0.2203	6	$SrCl_2$	0.0862	0.0223	2
$SrCl_2 \cdot 6H_2O$	0.2294	6	$SrCl_2$	0.0862	0.0239	2
$SrCl_2 \cdot 6H_2O$	0.2294	6	$SrCl_2$	0.0862	0.0239	5
$SrCl_2 \cdot 6H_2O$	0.2258	6	$SrCl_2$	0.0862	0.0233	6
$SrI_2 \cdot H_2O$		1			0.0219	4
$SrI_2 \cdot 2H_2O$		2			0.0232	4
$SrI_2 \cdot 6H_2O$		6			0.0241	4
$UO_2Cl_2 \cdot H_2O$	0.1378	1	UO_2Cl_2	0.1049		2
$UO_2Cl_2 \cdot 3H_2O$	0.1853	3	UO_2Cl_2	0.1049	0.0268	2
$UO_2SO_4 \cdot 5/2H_2O$	0.1912	2.5	UO_2SO_4 4	0.1206	0.0282	2
$UO_2SO_4 \cdot 7/2H_2O$	0.2019	3.5	UO_2SO_4	0.1206	0.0232	2
$UO_2SO_4 \cdot 3H_2O$	0.1799	3	UO_2SO_4	0.1206	0.0197	2
$YbCl_3 \cdot 6H_2O$	0.2499	6	$YbCl_3$	0.0935	0.0261	5
$ZnSO_4 \cdot H_2O$	0.0884	1	$ZnSO_4$	0.0689	0.0196	2
$ZnSO_4 \cdot H_2O$	0.0931	1	$ZnSO_4$	0.0705	0.0226	5
$ZnSO_4 \cdot H_2O$	0.0931	1	$ZnSO_4$	0.0717	0.0214	6
$ZnSO_4 \cdot 6H_2O$	0.2162	6	$ZnSO_4$	0.0689	0.0246	2
$ZnSO_4 \cdot 6H_2O$	0.2160	6	$ZnSO_4$	0.0705	0.0242	5
$ZnSO_4 \cdot 7H_2O$	0.2421	7	$ZnSO_4$	0.0689	0.0247	2
$ZnSO_4 \cdot 7H_2O$	0.2446	7	$ZnSO_4$	0.0689	0.0251	2
$ZnSO_4 \cdot 7H_2O$	0.2440	7	$ZnSO_4$	0.0705	0.0248	5
$ZnSO_4 \cdot 7H_2O$	0.2423	7	$ZnSO_4$	0.0717	0.0244	6
$Zr(SO_4)_2 \cdot 4H_2O$	0.2107	4	$Zr(SO_4)_2$	0.1461	0.0162	6

Table S4: Formuka unit molecular volumes, V, of hydrates, anhydrates and of waters of crystallisation, $V_m(H_2O)$, for seven outliers. Data from Jenkins, Ponikvar-Svet and Liebman (4:green),[4] Mercury (2:gold),[2] and "HSC Chemistry 8" (5:blue).[5]

Hydrate	V_m/nm³	$n(H_2O)$	Anhydrate	V_m/nm³	$V_m(H_2O)$/nm³	Source
$Na_2CO_3 \cdot H_2O$		1			0.0311	4
$SrCl_2 \cdot H_2O$		1			0.0351	4
$NaClO_4 \cdot H_2O$	0.1154	1	$NaClO_4$		0.0348	2
$AlCl_3 \cdot 6H_2O$	0.1672	6	$AlCl_3$	0.0893	0.0130	5
$La_2(SO_4)_3 \cdot 9H_2O$		9			0.0181	4
$La_2(SO_4)_3 \cdot 9H_2O$	0.4287	9	$La_2(SO_4)_3$	0.2610	0.0186	5
$Hg(NO_3)_2 \cdot H_2O$	0.1323	1	$Hg(NO_3)_2$	0.1253	0.0070	6

Table S5: $\Delta_r G$ / kJ mol^{-1} for 50 reactions under ambient conditions:[5]

parent + $n(H_2O(g))$ -> parent·nH_2O

parent·nH_2O	$n(H_2O)$	parent	$\Delta_r G$ / kJ mol^{-1}
$ZnSO_4·H_2O$	1	$ZnSO_4$	-34.69
$Al_2O_3·H_2O$	1	Al_2O_3	-31.18
$SrBr_2·H_2O$	1	$SrBr_2$	-27.39
$LiI·2H_2O$	2	LiI	-26.84
$FeSO_4·H_2O$	1	$FeSO_4$	-25.80
$LiI·3H_2O$	3	LiI	-25.32
$CuSO_4·H_2O$	1	$CuSO_4$	-23.98
$BaI_2·2H_2O$	2	BaI_2	-22.21
$MnSO_4·H_2O$	1	$MnSO_4$	-21.45
$Zr(SO_4)_2·4H_2O$	4	$Zr(SO_4)_2$	-21.26
$CaBr_2·6H_2O$	6	$CaBr_2$	-19.49
$BeSO_4·4H_2O$	4	$BeSO_4$	-19.18
$MgSO_4·6H_2O$	6	$MgSO_4$	-18.87
$CaSeO_4·2H_2O$	2	$CaSeO_4$	-18.69
$MgSO_4·7H_2O$	7	$MgSO_4$	-17.63
$CdSO_4·H_2O$	1	$CdSO_4$	-17.56
$CdSO_4·H_2O$	1	$CdSO_4$	-17.56
$CuSO_4·3H_2O$	3	$CuSO_4$	-17.40
$SrBr_2·6H_2O$	6	$SrBr_2$	-17.09
$UO_2SO_4·3H_2O$	3	UO_2SO_4	-15.85
$Li_2SO_4·H_2O$	1	Li_2SO_4	-15.72
$NiSO_4·6H_2O$	6	$NiSO_4$	-15.54
$CuSO_4·5H_2O$	5	$CuSO_4$	-14.95
$NiSO_4·7H_2O$	7	$NiSO_4$	-14.55
$CoBr_2·6H_2O$	6	$CoBr_2$	-14.48
$Ba(OH)_2·8H_2O$	8	$Ba(OH)_2$	-14.14

$Al_2O_3 \cdot 3H_2O$	3	Al_2O_3	-14.03
$ZnSO_4 \cdot 6H_2O$	6	$ZnSO_4$	-13.99
$CoSO_4 \cdot 6H_2O$	6	$CoSO_4$	-13.60
$Na_2B_4O_7 \cdot 10H_2O$	10	$Na_2B_4O_7$	-13.44
$ZnSO_4 \cdot 7H_2O$	7	$ZnSO_4$	-13.36
$KAl(SO_4)_2 \cdot 12H_2O$	12	$KAl(SO_4)_2$	-13.17
$BaBr_2 \cdot 2H_2O$	2	$BaBr_2$	-13.15
$CoSO_4 \cdot 7H_2O$	7	$CoSO_4$	-12.99
$LiBr \cdot 2H_2O$	2	LiBr	-12.61
$NaI \cdot 2H_2O$	2	NaI	-12.21
$Na_3PO_4 \cdot 12H_2O$	12	Na_3PO_4	-10.93
$MnSO_4 \cdot 4H_2O$	4	$MnSO_4$	-10.89
$Na_2CO_3 \cdot H_2O$	1	Na_2CO_3	-10.67
$MnSO_4 \cdot 5H_2O$	5	$MnSO_4$	-10.65
$Na_2S_2O_3 \cdot 5H_2O$	5	$Na_2S_2O_3$	-10.65
$NaBr \cdot 2H_2O$	2	NaBr	-9.97
$Na_2CO_3 \cdot 10H_2O$	10	Na_2CO_3	-9.50
$MnSO_4 \cdot 7H_2O$	7	$MnSO_4$	-9.47
$CaSO_4 \cdot 2H_2O$	2	$CaSO_4$	-9.16
$FePO_4 \cdot 2H_2O$	2	$FePO_4$	-9.03
$FePO_4 \cdot 2H_2O$	2	$FePO_4$	-9.03
$Na_2SO_4 \cdot 10H_2O$	10	Na_2SO_4	-9.00
$Na_2SO_3 \cdot 7H_2O$	7	Na_2SO_3	-8.86
$Na_2CO_3 \cdot 7H_2O$	7	Na_2CO_3	-8.67

References

1. Glasser, L., Water, water, everywhere - Phase diagrams of ordinary water substance. *J. Chem. Educ.* **2004,** *81*, 414-418.
2. Mercury, L.; Vieillard, P.; Tardy, Y., Thermodynamics of ice polymorphs and `ice-like' water in hydrates and hydroxides. *Appl. Geochem.* **2001,** *16*, 161-181.
3. Marcus, Y.; Jenkins, H. D. B., Standard absolute entropy, S_{298}^{o}, of salt hydrates from volumes and hydrate numbers and the thermodynamic difference rule. *Chem. Phys. Lett.* **2018,** *708*, 106-108.
4. Jenkins, H. D. B.; Ponikvar-Svet, M.; Liebman, J. F., Relative Packing Efficiency in Hydrates. *J. Chem. Eng. Data* **2009,** *54*, 2722-2728.
5. Outotec HSC Chemistry 8. http://www.outotec.com/en/Products--services/HSC-Chemistry/ (accessed April, 2019).
6. Yaws, C. L. Yaws' Thermophysical Properties of Chemicals and Hydrocarbons (Electronic Edition). https://app.knovel.com/hotlink/toc/id:kpYTPCHE02/yaws-thermophysical-properties/yaws-thermophysical-properties (accessed March, 2019).
7. ICSD Inorganic Crystal Structure Database. http://www2.fiz-karlsruhe.de/icsd_web.html (accessed April, 2019).
8. Sohr, J.; Schmidt, H.; Voigt, W., Higher hydrates of lithium chloride, lithium bromide and lithium iodide. *Acta Cryst. C* **2018,** *74*, 194-202.
9. Hennings, E.; Schmidt, H.; Voigt, W., Crystal structures of hydrates of simple inorganic salts. I. Water-rich magnesium halide hydrates $MgCl_2.8H_2O$, $MgCl_2.12H_2O$, $MgBr_2.6H_2O$, $MgBr_2.9H_2O$, $MgI_2.8H_2O$ and $MgI_2.9H_2O$. *Acta Cryst. C* **2013,** *69*, 1292-1300.
10. Hennings, E.; Schmidt, H.; Voigt, W., Crystal structures of hydrates of simple inorganic salts. II. Water-rich calcium bromide and iodide hydrates: $CaBr_2.9H_2O$, $CaI_2.8H_2O$, $CaI_2.7H_2O$ and $CaI_2.6.5H_2O$. *Acta Cryst. C* **2014,** *70*, 876-881.
11. Schmidt, H.; Hennings, E.; Voigt, W., Crystal structures of hydrates of simple inorganic salts. III. Water-rich aluminium halide hydrates: $AlCl_3.15H_2O$, $AlBr_3.15H_2O$, $AlI_3.15H_2O$, $AlI_3.17H_2O$ and $AlBr_3.9H_2O$. *Acta Cryst. C* **2014,** *70*, 882-888.