SUPPLEMENTARY INFORMATION

JESS, a Joint Expert Speciation System – VI: Thermodynamically-consistent Standard Gibbs Energies of Reaction for Aqueous Solutions

Peter M May and Darren Rowland

Chemistry, School of Engineering and Information Technology, Murdoch University,
Murdoch, WA 6150, Australia

Illustrative Examples

The following examples show how the new database can be used in practice. They can, however, only provide a glimpse of conceivable applications given the size of the data set and the complexity of reaction permutations.

Models are representations of reality which should always be designed to answer specific questions. Modellers should be aware that, if the intent of a thermodynamic calculation is to obtain quantitative information, few chemical systems are well enough experimentally characterised.[2] Usually, a narrower aim is to identify the predominant chemical species under given circumstances and hence to understand how the system is likely to respond to changing conditions.

In this context, the new facilities (as with other parts of JESS) are a tool for dealing with the pervasive and often remarkably large uncertainties which afflict thermodynamic data. Exact calculations always depend on a critical selection of parameters. This easily gives an impression of accuracy which is unwarranted, not only because of the subjectivity involved when choices are made but also because relatively few experimental measurements are ever confirmed independently.[2] Best practice thermodynamic modelling explores these limitations and describes the extent to which confidence in the results is justified. Support for such analyses is the key benefit of the present work.

To illustrate this, Table S1 considers certain organic metal-complexing reagents appearing for their laboratory relevance in the 'Handbook of Chemical Equilibria in Analytical Chemistry' by Kotrly and Sucha.[27] Table S2 shows how inconsistencies develop, and how they are resolved, when an increasing number of reactions in linear combination are needed to characterise non-basis species. Table S3 documents a case in which several older but widely-used references are superseded. Table S4 addresses a set of recently-published[28] solubility products, clearly illustrating the significant uncertainties which still prevail in this area.

Table S1. Stability constants, $\log_{10} K_{ML}^{0} = \frac{\{ML\}}{\{M\}.\{L\}}$, calculated in this work from relative species Gibbs energies[a], G^0, for the 1:1 metal-ligand complexing reactions (M + L ⇌ ML) of selected reagents as described in the text.

Reagent		**$\log_{10} K_{ML}^{0}$**					
	JESS symbol for L[b]	**JESS symbol for M[c]**					
		Cu+2	Fe+3	Fe+2	Ni+2	Pb+2	Zn+2
Trimethylenediamine 1,3-Propanediamine	13PrDiAm	9.702			6.419		
Dipicolinic acid 2,6-Pyridinedicarboxylic acid	26PyridineDiCOO-2	10.10			7.896	9.604	7.908
Neocuproine 2,9-Dimethyl-1,10-phenanthroline	29DiMePhenanth	5.215			5.000		4.100
Anthranilic acid 2-Aminobenzoic acid	2AmBenz-1	4.542			2.120	2.820	2.570
2-Chloro-1,10-phenanthroline	2ClPhenanth	5.145			4.580		3.300
Quinaldic acid 2-Quinolinecarboxylic acid	2QuinCOO-1	5.910		3.920	4.640	4.323	4.170
HTTA 2-Thenoyltrifluoroacetone 4,4,4-Trifluoro-1-(2-thienyl)-1,3-butanedione	2ThenTriFAcone-1	6.279	7.612		5.049		
4,7-Dimethyl-1,10-phenanthroline	47DiMePhenanth	8.760		5.600	8.440		6.420
5,6-Dimethyl-1,10-phenanthroline	56DiMePhenanth	8.710		6.342	8.250		6.870
5-Methyl-1,10-phenanthroline	5MePhenanth	8.550		6.321	8.300		6.620

5-Nitro-1,10-phenanthroline	5NitrPhenanth	8.000		5.473	7.000		5.400
Acetylacetone 2,4-Pentanedione	Acac-1	8.494	10.33	5.106	5.955	4.998	5.172
Adipic acid Hexanedioic acid; 1,4-Butanedicarboxylic acid	Adipic-2	3.157			2.186	3.905	2.685
L-Alanine 2-Aminopropanoic acid	Ala-1	8.568	10.60	4.533	5.843	5.618	5.192
L-Asparagine 2-Aminobutanedioic acid-4-amide	Asn-1	8.276	9.370	3.696	6.015	4.194	4.863
L-Aspartic acid 2-Aminobutanedioic acid	Asp-2	9.748	13.09	6.170	8.093	7.110	6.662
Benzoic acid	Benzoic-1	2.111	5.964		1.484	2.564	1.536
Bipyridyl 2,2'-Bipyridine 2-(2-Pyridyl)pyridine	Bipy	8.033		4.188	7.092	2.919	5.186
Catechol 1,2-Benzenediol	Cat-2	14.72	21.34	8.614	9.663	12.99	10.36
CDTA N,N'-(1R,2R)-1,2-cyclohexanediylbis[N-(carboxymethyl)glycine 1,2-Cyclohexylene- dinitrilotetraacetic acid	CDTA-4	22.88	32.19	20.02	21.89	21.42	20.47
Citric acid 2-Hydroxy-1,2,3-propanetricarboxylic acid	Citric-3	6.944	13.33	5.861	6.711	6.211	6.237
Chloroacetic acid	ClAcet-1	1.974	2.899			1.701	1.279

Diethylenetriamine N^1-(2-Aminoethyl)-1,2-ethanediamine 2,2'-Iminobis(ethylamine)	Dien	15.92		6.218	10.62	7.456	8.809
Dimethylglycine N,N-Dimethyl-2-aminoethanoic acid	DMG-1	7.608			5.190	7.546	4.136
DTPA Diethylene trinitrilotetraacetic acid N,N-bis[2-[bis(carboxymethyl)amino]ethyl]glycine	DTPA-5	23.43	30.38	18.58	22.17	20.62	20.14
EDTA Ethylenediaminetetraacetic acid N,N'-1,2-ethanediylbis[N-(carboxymethyl)glycine	EDTA-4	20.40	27.43	15.88	20.14	19.70	18.22
EGTA Ethylene-bis(oxyethylenenitrilo) tetraacetic acid 3,12-bis(carboxymethyl)-6,9-dioxa-3,12-diazatetradecanedioic acid	EGTA-4	19.24	23.00	13.47	15.22	16.31	14.42
Ethylenediamine 1,2-Diaminoethane 1,2-Ethanediamine	EtDiAm	10.50		4.321	7.412	5.035	5.738
Ethanolamine 2-Aminoethanol	EtOlAm	4.537		1.610	3.083	4.106	2.519
Formic acid Methanoic acid	Formic-1	2.134	2.523		1.199	1.838	1.412
Fumaric acid 2-Butenedioic acid (2E)	Fumaric-2	2.574	3.248		2.506	3.006	2.332
Glutamic acid 2-Aminopentanedioic acid	Glu-2	9.127	13.51	4.471	6.377	5.947	5.825
Glycine 2-Aminoethanoic acid	Gly-1	8.573	11.35	4.303	6.176	5.310	5.431

Glycolic acid 2-Hydroxyethanoic acid 2-Hydroxyacetic acid	Glycolic-1	3.001	3.700	1.900	3.387	2.441	2.577
Glycylglycine Diglycine	GlyGly-1	6.041	9.300	2.700	4.416	3.752	3.945
Glycylglycylglycine Triglycine	GlyGlyGly-1	5.691			4.139	3.683	3.538
Glycylglycylglycylglycine Tetraglycine	GlyGlyGlyGly-1	5.527			4.062	3.606	3.570
Glycinamide Aminoethanoic acid amide 2-Aminoacetamide	GlyNH2	5.354			4.093		3.280
Hydroxyethylethylenediamine 2-(2-Aminoethylamino)ethanol	HEEN	10.05			6.821	5.58	5.015
HOEDTA N-(2-Hydroxyethyl)ethylene diaminetriacetic acid N-[2-[bis(carboxymethyl)amino]ethyl]-N-(2-hydroxyethyl)glycine	HOEDTA-3	18.76	21.71	12.92	18.16	16.11	15.75
Iminodiacetic acid N-(Carboxymethyl)glycine	IDA-2	11.38	12.30	6.625	8.973	8.227	8.011
Imidazole 1,3-Diazole	Imidazole	4.234		1.806	3.048	0.500	2.534
Kojic acid 5-Hydroxy-2-hydroxymethyl-4H-pyran-4-one	Kojic-1	7.010	9.526		5.312		5.398
Lactic acid 2-Hydroxypropanoic acid	Lactic-1	2.752	4.720	1.980	2.024	2.590	2.311
L-Leucine 2-Amino-4-methylpentanoic acid	Leu-1	8.689	7.840	3.940	5.921	5.516	5.143

Maleic acid cis-1,2-Ethylenedicarboxylic acid 2-Butenedioic acid (2Z)	Maleic-2	4.334	7.248		2.716	4.068	2.840
Malic acid Hydroxyethane-1,2-dicarboxylic acid 2-Hydroxybutanedioic acid	Malic-2	4.364	8.271	3.402	3.918	3.231	3.772
Malonic acid 1,3-Propanedioic acid	Malonic-2	5.880	9.349	2.801	4.079	4.200	3.789
Mandelic acid 2-Phenyl-2-hydroxyethanoic acid α-Hydroxybenzeneacetic acid	Mandelic-1	3.253			2.463		2.420
MIDA N-Methyliminodiethanoic acid N-(Carboxymethyl)-N-methylglycine	MIDA-2	11.89	12.77	7.510	9.497	8.800	8.491
L-Norvaline 2-Aminopentanoic acid	Norval-1	8.601			5.824		4.865
NTA Nitrilotriacetic acid Nitrilotriethanoic acid N,N-Bis(carboxymethyl)glycine	NTA-3	14.26	18.04	9.924	12.65	12.66	11.74
NTMP Nitrilotris(methylene)triphosphonic acid P,P',P''-[Nitrilotris(methylene)]trisphosphonic acid	NTMP-6	19.40		16.00	14.20		17.10
Oxalic acid Ethanedioic acid	Oxalic-2	6.119	9.499	3.634	5.302	5.166	4.743
Oxine 8-Hydroxyquinoline 8-Quinolinol	Oxine-1	12.32	14.24		9.579	9.218	8.748

PAR 4-(2-Pyridylazo)resorcinol 4-[2-(2-Pyridinyl)diazenyl]-1,3-benzenediol	PAR-2	18.08			14.88		12.03
1,10-Phenanthroline	Phenanth	9.036		5.793	8.588		6.419
Phenylthioacetic acid S-Phenylmercaptoethanoic acid 2-(Phenylthio)acetic acid	PhenThioAcet-1	1.918			1.118	2.216	1.216
Phthalic Acid 1,2-Benzenedicarboxylic acid	Phthalic-2	4.110			3.029	4.244	2.972
Picolinic acid 2-Pyridinecarboxylic acid	Picolinic-1	8.464	6.908	5.348	7.036	5.115	5.613
Pimelic acid 1,7-Heptanedioic acid	Pimelic-2	3.042			2.032	3.452	2.132
Phosphoserine O-Phosphono-L-serine	PO4Ser-3	10.94	16.20		7.813		7.188
L-Proline Pyrrolidine-2-carboxylic acid	Pro-1	9.281	10.70	4.600	6.382	4.480	5.745
Pyridine	Pyridine	2.512		0.600	1.834		1.025
Pyruvic acid 2-Oxopropanoic acid	Pyruvic-1	2.435	4.720	1.187	1.860	2.854	2.023
Salicylaldehyde 2-Hydroxybenzaldehyde	SalAld-1	5.986	9.246		4.161	3.632	3.462
Salicylic acid 2-Hydroxybenzoic acid	Salicylic-2	11.55	17.67	7.273	7.771	6.460	7.542
Sarcosine N-Methyl-2-aminoethanoic acid N-Methylglycine	Sar-1	8.275			5.858		4.910

Succinic acid 1,4-Butanedioic acid	Succinic-2	3.359	9.141	2.385	2.441	3.792	2.705
Sulfoxine 8-Hydroxyquinoline-5-sulfonic acid	Sulfox-2	12.87	13.07		9.836	8.527	8.954
Sulfosalicylic acid 3-Carboxy-4-hydroxybenzenesulphonic acid 2-Hydroxy-5-sulfobenzoic acid	SulfSal-3	10.74	16.58	6.143	7.833		9.767
5-Sulfosalicylaldehyde 3-Formyl-4-hydroxybenzenesulfonic acid	SulfSalAld-2	5.960			4.446		3.648
Tartaric acid 2,3-Dihydroxybutanedioic acid	Tartaric-2	4.072	6.990	3.399	3.781	3.833	3.580
Tetraethylenepentamine 3,6,9-Triazaundecane-1,11-diamine N1-(2-Aminoethyl)-N2-[2-[(2-aminoethyl)amino]ethyl]-1,2-ethanediamine	Tetren	24.07		9.850	17.47	10.41	15.21
Thiourea Thiocarbamide	Thiourea	5.700				0.354	-0.705
Tiron Catechol-3,5-disulphonic acid 4,5-Dihydroxy-1,3-benzenedisulfonic acid	Tiron-4	16.03	22.88		11.61	14.09	12.11
Triaminotriethylamine Nitrilotris(2-ethylamine) N1,N1-Bis(2-aminoethyl)-1,2-ethanediamine	Tren	18.84		8.697	14.56		14.49
Triethylenetetramine 1,2-Diamino-N,N'-di(2-aminoethyl)ethane N1,N2-Bis(2-aminoethyl)-1,2-ethanediamine	Trien	20.01		7.620	13.98	10.32	11.53
Triethanolamine 2,2',2''-Nitrilotriethanol	TriEtOlAm	4.099	7.000	2.270	2.782	3.390	1.904

Tris THAM 2-Amino-2-(hydroxymethyl)-1,3-propandiol	Tris	4.006			2.656	2.700	2.240
Tropolone 1-Hydroxycyclohepta-3,5,7-trien-2-one 2-Hydroxy-2,4,6-cycloheptatrien-1-one	Tropolone-1	8.766	11.23		6.386		6.256
TTHA Triethylenetetraaminehexaethanoic acid 3,6,9,12-Tetrakis(carboxymethyl)-3,6,9,12-tetraazatetradecanedioic acid	TTHA-6	24.32	31.44	19.60	21.23	20.54	20.65

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[a] In exact agreement with values obtained from the JPD database in all cases except Fe+3/PO4Ser-3 (16.14 *c.f.* 16.20), Zn+2/PAR-2 (12.38 *c.f.* 12.03) and Cu+2/2ClPhenanth (5.070 *c.f.* 5.145)

[b] Charges on each ligand L, where applicable, occur at the end of each JESS symbol preceded by the negative sign.

[c] Charges on each metal ion M occur at the end of each JESS symbol preceded by the positive sign.

Table S2. Numerical analysis of EDTA protonation reactions: An example of how thermodynamic inconsistencies develop and how they are resolved by the ordered Gaussian elimination process.

JPD no.	**Reaction in JESS format**	**IC**[a]	**JPD**[b] **lgK^0**	**LC**[c] **lgK^0**	**This work**[d]
13	H+1 + EDTA-4 = H+1_EDTA-4	184	11.04	11.04	11.04
14	H+1_EDTA-4 + H+1 = H+1(2)_EDTA-4	236	6.801	6.801	6.801
15	H+1(2)_EDTA-4 + H+1 = H+1(3)_EDTA-4	137	3.154	3.154	3.154
1924	2<H+1> + EDTA-4 = H+1(2)_EDTA-4	33	16.87[e]	17.84	17.84[f]
1925	3<H+1> + EDTA-4 = H+1(3)_EDTA-4	21	20.72	21.00	21.00[f]

[a] Information content of the reaction (as described in the appendix).

[b] lgK^0 from the JPD database

[c] lgK^0 from the linear combination of reactions determined by ordered Gaussian elimination. Reactions 13, 14 and 15 (with highest IC) are used directly or in linear combination where applicable (i.e. to determine lgK^0 for reactions 1924 and 1925).

[d] Calculated from the relative Gibbs energies (kJ mol^{-1}) of the non-basis species:
H+1_EDTA-4 (–63.025); H+1(2)_EDTA-4 (–101.84); H+1(3)_EDTA-4 (–119.85).
The basis species are H+1 and EDTA-4.

[e] A value that is evidently too low, arising from inaccurate estimates in the literature, almost certainly attributable to the effect of Na^+ in the background electrolyte not being taken properly into account. Literature lgKs come from Morel and Hering[6] (17.18 at infinite dilution) and others either at low ionic strength where the medium is unspecified / considered 'Inert' or at 37 °C. More satisfactorily, reactions 13-15 have lgKs measured in KNO_3(aq) at 20 and 25 °C. The MINTEQA2 value[28] for infinite dilution at 25 °C (16.21) was not included (Weight=0).

[f] Bypassing the errors from reactions 1924 and 1925, reactions which are found to be redundant.

Table S3. A fully-worked example where several authoritative but out-of-date values have been superseded.

Summary

For $Ag(CN)_2^-$ + e^- $\rightleftharpoons$ Ag(s) + $2CN^-$ (JPD reaction 57,568), some widely-used sources all give E^0 = –0.310 V (equivalent to lgK^0 = –5.24 or $\Delta_{rxn}G^0$ = 29.1 $kJ.mol^{-1}$). However, the preferred value from the present work is E^0 = –0.419 V (equivalent to lgK^0 = –7.09 or $\Delta_{rxn}G^0$ = 40.47 $kJ.mol^{-1}$).

This result is obtained from the values for $Ag+1\_(CN^-)_2$ $\rightleftharpoons$ $2CN^-$ + Ag^+ (JPD reaction 55,463 **reversed**) with lgK^0 = –20.64 or $\Delta_{rxn}G^0$ = 117.8kJ.mol^{-1} in linear combination with Ag^+ + e^- $\rightleftharpoons$ Ag(s) with E^0 = 0.776 V equivalent to lgK^0 = 13.55 or $\Delta_{rxn}G^0$ = –77.33 $kJ.mol^{-1}$.

Raw data from the JPD database

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Reaction No. 57,568
Ag+1_CN-1(2) + e-1 = Ag(s) + 2<CN-1>
1 t=25 I=0 Inf. Dilution                              lgK -7.1(2SF) Wgt=1 ESC[]
2 t=25 I=0 Inf. Dilution                       lgK -6.9(0.05SD) Wgt=0 ENS[5569]
3 t=25 I=0 Inf. Dilution                            E -0.31(2SF) Wgt=0 MAG[778]
4 t=25 I=0 Inf. Dilution                           E -0.31(2SF) Wgt=0 CRV[3006]
5 t=25 I=0 Inf. Dilution                           E -0.31(2SF) Wgt=0 ENS[7276]
6 t=25 I=0 Inf. Dilution                          E -0.31(2SF) Wgt=0 CRV[22551]

Reaction No. 55,463
2<CN-1> + Ag+1 = Ag+1_CN-1(2)
1 t=15 I=0.1 Unknown                             lgK 21.38(4SF) Wgt=4 MIS[5872]
2 t=20 I=0.1 AgNO3                            lgK 20.45(0.07SD) Wgt=5 MIS[4593]
3 t=20 I=0.1 KNO3                                lgK 18.75(4SF) Wgt=0 MIS[6742]
4 t=20.5 I=0 Inf. Dilution                     lgK 20.85(0.01SD) Wgt=4 MGL[222]
5 t=21 I=3.25 NaClO4                            lgK 20.2(0.06SD) Wgt=5 MHG[222]
6 t=25 I=0 Inf. Dilution                             lgK 20.73(4SF) Wgt=1 EOR[]
7 t=25 I=0 Inf. Dilution                          lgK 20.48(4SF) Wgt=4 CRV[552]
8 t=25 I=0 Inf. Dilution                        lgK 21.99(4SF) Wgt=3 MGL[6140]<
9 t=25 I=0 Inf. Dilution                          lgK 20.5(3SF) Wgt=4 ENS[6405]
10 t=25 I=0 Inf. Dilution                         lgK 21.0(3SF) Wgt=0 CRV[8693]
11 t=25 I=0 CN- salt                              lgK 20.9(3SF)w Wgt=3 MPH[884]
12 t=25 I=1 NaClO4                            lgK 20.14(0.05SD) Wgt=5 MGL[5933]
13 t=30                                           lgK 21.1(3SF) Wgt=0 MHG[5873]
14 t=25 I=0 Inf. Dilution                        dH -32.7(0.2SD) Wgt=4 ENS[766]
15 t=25 I=0 Inf. Dilution                       dH -32.9(0.1SD) Wgt=4 MCL[4915]
16 t=25 I=0 Inf. Dilution                        dH -34.(0.3SD) Wgt=4 MCL[5326]
17 t=25 I=0 Inf. Dilution                    dH -140.2(1.2SD)kJ Wgt=5 MCL[6140]
18 t=25 I=1 NaCl                                dH -34.5(0.2SD) Wgt=5 MCL[5326]
19 t=25 I=1 NaClO4                           dH -144.2(0.9SD)kJ Wgt=3 MCL[6140]
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Fitted data from JPD reaction 55,463

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                                                                         Residual
                                                                        (weighted)
10 t=25 I=0 Inf. Dilution                    lgK 21.0 Wgt=0[8693]           0.36
3 t=20 I=0.1 KNO3                           lgK 18.75 Wgt=0[6742]           -2.1
12 t=25 I=1 NaClO4                           lgK 20.1 Wgt=5[5933]       -0.00085
5 t=21 I=3.25 NaClO4                          lgK 20.2 Wgt=5[222]         0.0012
19 t=25 I=1 NaClO4                          dH -34.5 Wgt=3[6140]         -0.043
6 t=25 I=0 Inf. Dilution                       lgK 20.73 Wgt=1[0]          0.094
18 t=25 I=1 NaCl                            dH -34.5 Wgt=5[5326]         -0.079
17 t=25 I=0 Inf. Dilution                   dH -33.5 Wgt=5[6140]          -0.18
1 t=15 I=0.1 Unknown                        lgK 21.38 Wgt=4[5872]           0.12
9 t=25 I=0 Inf. Dilution                     lgK 20.5 Wgt=4[6405]          -0.14
7 t=25 I=0 Inf. Dilution                     lgK 20.48 Wgt=4[552]          -0.16
15 t=25 I=0 Inf. Dilution                   dH -32.9 Wgt=4[4915]           0.43
4 t=20.5 I=0 Inf. Dilution                    lgK 20.9 Wgt=4[222]          -0.16
11 t=25 I=0 CN- salt                          lgK 20.9 Wgt=3[884]           0.26
14 t=25 I=0 Inf. Dilution                     dH -32.7 Wgt=4[766]           0.63
16 t=25 I=0 Inf. Dilution                   dH -34.0 Wgt=4[5326]          -0.67
2 t=20 I=0.1 AgNO3                           lgK 20.5 Wgt=5[4593]          -0.38
8 t=25 I=0 Inf. Dilution                    lgK 21.99 Wgt=3[6140] >          1.4
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Table S4. Some recently-reported solubility products with an analysis exposing the uncertainty that still prevails in this work and other applications.

Solid	**$\log_{10}K_S$[a]**	**logK (this work)**	**logK (JPD)**
$Na_2SO_4.10H_2O$	–1.219[b]	–1.310[d]	–1.228[j]; –1.18[k]
Na_2SO_4	–0.255[b]	–0.372[e,f]	–0.287[j]; –0.27[k] –0.33[l]
K_2SO_4	–1.792[b]	–1.822[e,g]	–1.776[j]; –1.76[k]; –1.77[m]; –1.85[n]
$NaBr.2H_2O$	2.017[c]	–0.345[h]	N/A
KBr	1.141[c]	1.095[e,i]	1.13[k]; 1.129[o]; 1.145[p]

[a] Rounded value as selected by Cui et al.[28]

[b] Citing J.P. Greenberg and N. Møller, *Geochim. Cosmochim. Acta*, 1989, 53, 2503-2518.

[c] Citing C. Christov, *Geochim. Cosmochim. Acta*, 2007, 71, 3557-3569..

[d] Based on numerously-reported values of $\Delta_f G_m^0$ = –3646.9 kJ.mol^{-1} (in appropriate linear combination).

[e] Based on value (in appropriate linear combination) from several sources but mainly I. Barin and G. Platzki, "Thermochemical Data of Pure Substances, 3rd Edn." Weinheim, Germany, 1995.

[f] $\Delta_f G_m^0$ = –1271.9 kJ.mol^{-1}

[g] $\Delta_f G_m^0$ = –1322.4 kJ.mol^{-1}

[h] Based on value of $\Delta_f G_m^0$ = –838.2 kJ.mol^{-1} (in appropriate linear combination) from G.P. Thiel and J.H. Lienhard V, *Desalination*, 2014, 346, 54-69.

[i] $\Delta_f G_m^0$ = –380.7 kJ.mol^{-1} (with exact agreement between I. Barin and G. Platzki, "Thermochemical Data of Pure Substances, 3rd Edn." Weinheim, Germany, 1995, R.A. Robie and B.S. Hemingway, "U.S. Geol. Surv. Bull. 2131, Thermodynamic Properties of Minerals and Related Substances at 298.15 K and 1 Bar (10^5 Pascals) Pressure and at Higher Temperatures" U.S. Government Printing Office, Washington, U.S.A, 1995 and other secondary sources).

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