

## Hexary System of Oceanic Salts – Polythermal Pitzer Dataset (numerical supplement)

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**Abstract:** For the polythermal Pitzer dataset of the hexary system of oceanic salts ( $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Cl}^-$ ,  $\text{SO}_4^{2-}$  -  $\text{H}_2\text{O}$ ) including acids and hydroxides the data selection is documented in detail in the report “THEREDA - Thermodynamische Referenzdatenbasis” (Altmaier et al. 2011, <https://www.grs.de/de/aktuelles/publikationen/grs-265-thereda-thermodynamische-referenzdatenbasis-abschlussbericht>).

The present short communication supplements this report by the numerical values of all temperature coefficients.

Part of the process to assess the safety of disposal sites for radioactive or chemical-toxic waste is the predictive modelling of the solubility of hazardous components in a complex aqueous solution. In the case of the host rock salt, the major ions of the solutions are those of the hexary system  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Cl}^-$ ,  $\text{SO}_4^{2-}$  -  $\text{H}_2\text{O}$ , which form the oceanic salts. For consideration of pH variations, the corresponding acidic ( $\text{HCl}$ ,  $\text{H}_2\text{SO}_4$ ) and basic ( $\text{NaOH}$ ,  $\text{KOH}$ ,  $\text{Mg}(\text{OH})_2$ ,  $\text{Ca}(\text{OH})_2$ ) systems are included (cf. Tab. 1).

The Pitzer dataset was developed based on the data set of [HAR/MOL1984] (HMW model). While the HMW model is only valid at 25 °C, THEREDA is the first database for the temperature range from 0–100 °C. Data selection and parametrisation is documented in [ALT/BRE2011] (pp. 233 to 301). The report presents all data sources, fitting equations and procedures as well as numerous graphical comparisons of experimental and calculated data (graphics are also available on the THEREDA website under Application Examples). However, no tabulation of the final numerical values of the

database is included. In Tables 1 to 4 of this short communication the values are now listed in addition.

### References

[ALT/BRE2011] Altmaier, M., Brendler, V., Bube, C., Marquardt, C., Moog, H. C., Richter, A., Scharge, T., Voigt, W., Wilhelm, S., Wilms, T., Wollmann, G.: THEREDA - Thermodynamische Referenzdatenbasis. Ed.: GRS Report No. 265, Köln (2011).

[HAR/MOL1984] Harvie, C. E., Møller, N., Weare, J. H.: The prediction of mineral solubilities in natural waters: Na-K-Mg-Ca-H-Cl-SO<sub>4</sub>-OH-HCO<sub>3</sub>-CO<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system to high ionic strengths at 25 °C. *Geochimica et Cosmochimica Acta* 48 (1984) pp. 723–751.

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**Tab. 1:** Temperature coefficients for the standard Gibbs energy,  $\Delta_R G^\circ$  for formation of species or phases from ions and water. Note that in THEREDA for all Primary Master species  $\Delta_R H_{i,T=T_0}^\circ$ ,  $S_{i,T=T_0}^\circ$  and thus  $\Delta_R G_{i,T=T_0}^\circ = 0$ .

$$\Delta_R G^\circ = A + B \cdot T + C \cdot T \cdot \ln(T) + D \cdot T^2 + E \cdot T^3 + \frac{F}{T}$$

Formula	Mineralname (if existing)	Tmin/K	Tmax/K	A	B	C	D	E	F
H2O		273.15	393.15	0	0	0	0	0	0
H+		273.15	393.15	0	0	0	0	0	0
Na+		273.15	393.15	0	0	0	0	0	0
K+		273.15	393.15	0	0	0	0	0	0
Mg+2		273.15	393.15	0	0	0	0	0	0
Ca+2		273.15	393.15	0	0	0	0	0	0
Cl-		273.15	393.15	0	0	0	0	0	0
SO4-2		273.15	393.15	0	0	0	0	0	0
OH-		273.15	523.15	977916.173	-24698.7262	4264.428838	-8.43137921	0.003231957	-34104000
KMg(SO4)+		298.15	393.15	103945	-300	0	0	0	0
Ca(SO4)(aq)		273.15	393.15	0	215.4333318	0	-0.666666662	0	0
KCa(SO4)+		298.15	393.15	15957.55	-77	0	0	0	0
HSO4-		273.15	373.15	-253892.5093	10767.94618	-1961.905733	4.74380171	-0.0021397	0
Mg(OH)+		273.15	373.15	4444044.0813	-5495.03903	798.7412063	0	-0.00052773	-24391000
Ca(OH)2	Portlandite	273.15	393.15	0	7181.2509495777	-1394.5143267856	4.80357314	-0.0025896965	0
Ca(SO4)	Anhydrite	293.15	383.15	-1634543.75318913	80144.23225363	-15209.01605	47.389963	-0.0249854497	0
Ca(SO4):0.5H2O		273.15	373.15	-4030000	196701.5735	-37230.0854	114.2701381	-0.05857491	0
Ca(SO4):2H2O	Gypsum	273.15	393.15	-2531757.2917543	124418.55047601	-23616.96979169	73.66531608	-0.0384455958	0
Ca2Cl2(OH)2:H2O		273.15	393.15	0	14792.223685972	-3037.5181297747	12.0591858867	-0.0064205121	0
Ca4Cl2(OH)6:13H2O		273.15	303.15	0	200912.75543616	-45011.75315	232.19009705	-0.13906309	0
CaCl2:6H2O	Antarcticite	273.15	300.15	-16325646.979329	412874.15944407	-70032.85829	121.51740047	-0.0318257	673905009.25962
K(HSO4)	Mercallite	273.15	348.15	-814526.581	15529.13293	-2368.04618	0	0.002737294	37827600

Tab. 1 (continued)

Formula	Mineralname (if existing)	Tmin/K	Tmax/K	A	B	C	D	E	F
K <sub>2</sub> Ca(SO <sub>4</sub> ) <sub>2</sub> :H <sub>2</sub> O	Syngenite	298.15	393.15	59721312.9236	-2893908.7268	546617.8335	-1662.21848	0.8397009377	0
K <sub>2</sub> Ca <sub>5</sub> (SO <sub>4</sub> ) <sub>6</sub> :H <sub>2</sub> O	Goergeyite	298.15	393.15	-511049.2208	11427.173794	-1789.808989	0	0	0
K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> :4H <sub>2</sub> O	Leonite	313.15	343.15	79692.2519	-1064.981273	0	3.827752933	-0.004721709514	0
K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> :6H <sub>2</sub> O	Picromerite	273.15	323.15	-29989.90633	17.6047585	0	0	0	0
K <sub>2</sub> Mg <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	Langbeinite	323.15	393.15	121025243.65	-2978817.11627	506347.42326	-941.62365	0.32892	-5383692863.79
K <sub>2</sub> MgCa <sub>2</sub> (SO <sub>4</sub> ) <sub>4</sub> :2H <sub>2</sub> O	Polyhalite	298.15	393.15	0	-683.2503053	0	3.003110928	-0.00542980206	0
K <sub>2</sub> SO <sub>4</sub>	Arcanite	273.15	423.15	-107917.5862	691.7215912	0	-1.503571476	0.0009507982006	0
K <sub>3</sub> (HSO <sub>4</sub> )(SO <sub>4</sub> )		273.15	348.15	-4881800	222927.8282	-41527.8943	116.5563335	-0.05358502	0
K <sub>4</sub> Mg <sub>4</sub> Cl <sub>4</sub> (SO <sub>4</sub> ) <sub>4</sub> :11H <sub>2</sub> O	Kainite	298.15	393.15	-44652402.06	2201390.673	-417522.5619	1298.101325	-0.6725960486	0
K <sub>6</sub> Na <sub>2</sub> (SO <sub>4</sub> ) <sub>4</sub>	Glaserite	273.15	393.15	0	-817.571878	0	3.735657062	-0.004970177043	0
K <sub>8</sub> (HSO <sub>4</sub> ) <sub>6</sub> (SO <sub>4</sub> )	Misenite	273.15	323.15	-20309.1795	0	0	-0.98371727	0.001775431	0
KCl	Sylvite	273.15	473.15	-162523.3941	5834.903636	-1043.271639	2.640137947	-0.0012970464	0
KMgCl <sub>3</sub> :6H <sub>2</sub> O	Carnallite	298.15	393.15	31505.27368	-2025.85817	399.7473724	-0.920702567	0	0
Mg(OH) <sub>2</sub>	Brucite	273.15	393.15	127348.8077	-99.3761865	0	0	0	0
Mg(SO <sub>4</sub> ):H <sub>2</sub> O	Kieserite	298.15	473.15	0	96.35534705	0	-0.2022853024	-0.0004318969955	0
Mg(SO <sub>4</sub> ):6H <sub>2</sub> O	Hexahydrite	273.15	393.15	0	-103.6553421	0	0.4963296291	-0.0008507834516	0
Mg <sub>2</sub> CaCl <sub>6</sub> :12H <sub>2</sub> O	Tachyhydrite	273.15	393.15	-480.8749209	-19188.22859	4771.001651	-33.74457936	0.0270397131	0
Mg <sub>7</sub> Na <sub>12</sub> (SO <sub>4</sub> ) <sub>13</sub> :15H <sub>2</sub> O	Loewite	298.15	393.15	-424299.6294	3324.129485	0	-7.084941358	0	0
MgCl <sub>2</sub> :6H <sub>2</sub> O	Bischofite	273.15	389.15	4095895.434	-195408.9322	36798.92745	-109.7047406	0.05399217544	0
MgNa <sub>6</sub> (SO <sub>4</sub> ) <sub>4</sub>	Vanthoffite	298.15	393.15	-56967.8992	612.343794	0	-1.498240746	0	0
Mg(SO <sub>4</sub> ):7H <sub>2</sub> O	Epsomite	273.15	343.15	0	-146.692199	0	0.6055492246	-0.0007859538299	0
Na(HSO <sub>4</sub> ):H <sub>2</sub> O		273.15	333.15	-4696.485816	-39915.83487	9446.267589	-61.26901723	0.0492147102	-179.3661932
Na <sub>2</sub> (SO <sub>4</sub> ):10H <sub>2</sub> O	Mirabilite	273.15	303.15	0	-538.4421493	0	2.545201591	-0.002743898333	0
Na <sub>2</sub> (SO <sub>4</sub> )	Thenardite	273.15	473.15	-74836.78364	1781.886588	-271.6978801	0.0390341458	0	0
Na <sub>21</sub> MgCl <sub>3</sub> (SO <sub>4</sub> ) <sub>10</sub>	Dansite	313.15	393.15	-3057443.503	26617.00896	0	-75.45150039	0.06914886934	0
Na <sub>2</sub> Ca(SO <sub>4</sub> ) <sub>2</sub>	Glauberite	298.15	373.15	-158818.59301554	3748.43953905	-581.93163569	0	0	0
Na <sub>2</sub> Ca <sub>5</sub> (SO <sub>4</sub> ) <sub>6</sub> :3H <sub>2</sub> O		308.15	348.15	-453127.21852381	10465.7897663	-1646.48296612	0	0	0
Na <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> :4H <sub>2</sub> O	Bloedite	273.15	393.15	-139697.3848	890.6725871	0	-1.566514441	0	0
Na <sub>3</sub> (HSO <sub>4</sub> )(SO <sub>4</sub> )		273.15	393.15	4712442.126	-220547.4568	41204.58816	-116.3552281	0.0523535563	0
Na <sub>4</sub> Ca(SO <sub>4</sub> ) <sub>3</sub> :2H <sub>2</sub> O	Labile-salt	298.15	348.15	-127642.36742584	3041.378905	-477.51957489	0	0	0
NaCl	Halite	273.15	393.15	7895365.369	-201321.2537	34480.30816	-66.76588747	0.02407524316	-339425117

Tab. 2: Temperature coefficients of the equation for the Pitzer parameter (binary).

$$P = \frac{a}{T} + b + c \cdot \ln(T) + d \cdot T + e \cdot T^2 + \frac{f}{T^2}$$

			<b>a</b>	<b>b</b>	<b>c</b>	<b>d</b>	<b>e</b>	<b>f</b>
Ca+2	Cl-	beta(0)	523608.18638425	-13074.636319461	2228.557995242	-4.1971890564676	0.0014752200493114	-22971638.598298
Ca+2	Cl-	beta(1)	0	3.478658161044	0	-0.015416814600998	0.000031790617595766	0
Ca+2	Cl-	Cphi	-49450.01852654	1237.2084127933	-210.95365351615	0.39806395333454	-0.0001401890552649	2165261.286
Ca+2	Cl-	alpha(1), alpha(2)	2	0				
Ca+2	HSO4-	beta(0)	988.07446509111	-42.190019472007	7.6242665704492	-0.014306066510313	0	0
Ca+2	HSO4-	beta(1)	0	91.863314703229	-19.068132359132	0.064205260809429	0	0
Ca+2	HSO4-	Cphi	0	0	0	0	0	0
Ca+2	HSO4-	alpha(1), alpha(2)	2	0				
Ca+2	OH-	beta(0)	415.17295604065	-1.5810565301582	0	0.00026407394395334	0	0
Ca+2	OH-	beta(1)	0	-0.2303	0	0	0	0
Ca+2	OH-	beta(2)	0	-5.72	0	0	0	0
Ca+2	OH-	Cphi	0	0	0	0	0	0
Ca+2	OH-	alpha(1), alpha(2)	2	50*				
Ca+2	SO4-2	beta(0)	55277.170954591	-2471.1092331818	457.9184134079	-1.2511930110049	0.00056153968969872	0
Ca+2	SO4-2	beta(1)	-80237.681510341	3589.7944058151	-665.41621490168	1.8400554958205	-0.00084165749112995	0
Ca+2	SO4-2	beta(2)	0	-227.91066053882	0	0.5813966191593	0	0
Ca+2	SO4-2	Cphi	0	0	0	0	0	0
Ca+2	SO4-2	alpha(1), alpha(2)	1.4	12				
H+	Cl-	beta(0)	9901.2219784713	-285.6473091587	50.067215202357	-0.10902829201997	0.000042832131817909	-351026.15442901
H+	Cl-	beta(1)	189788.67075591	-4588.8079271153	776.48444741115	-1.3963936941488	0.00046718218052799	-8599260.9958506
H+	Cl-	Cphi	0	0	0	0	0	0
H+	Cl-	alpha(1), alpha(2)	2	0				
H+	HSO4-	beta(0)	-3779.1070431174	118.05012777677	-21.070988995129	0.052015109988574	-0.00002399772686271	134621.0365025
H+	HSO4-	beta(1)	0	0.20249372758434	0	0.0016007779060677	-0.0000026845177100247	0
H+	HSO4-	Cphi	0	0	0	0	0	0
H+	HSO4-	alpha(1), alpha(2)	2	0				

Tab. 2 (continued)

			a	b	c	d	e	f
H+	SO4-2	beta(0)	18216.370413134	-565.47153166155	101.57210751098	-0.2634251798665	0.0001303524096458	-648886.46966143
H+	SO4-2	beta(1)	0	0	0	0	0	0
H+	SO4-2	Cphi	12441.700655481	-387.73249251308	69.37103031	-0.17062382103554	0.000075001664802453	-443201.09567623
H+	SO4-2	alpha(1), alpha(2)	2	0				
K+	Cl-	beta(0)	-758.47633050695	26.737234722473	-4.7061851476336	0.010071983860725	-0.0000037598981538277	0
K+	Cl-	beta(1)	112193.16841662	-2804.0348355283	478.32163208852	-0.90718308906128	0.00032392910397498	-4946661.7980636
K+	Cl-	Cphi	91.270112261712	-3.3052735859041	0.58644312766853	-0.0012980628672801	4.95707610920681E-07	0
K+	Cl-	alpha(1), alpha(2)	2	0				
K+	HSO4-	beta(0)	0	-0.00029999639184557	0	0	0	0
K+	HSO4-	beta(1)	0	0.012027181430032	0	0	0	0
K+	HSO4-	Cphi	7.1255733237116	-0.075207675506645	0	0.00022865325034578	-1.8366779120813E-07	0
K+	HSO4-	alpha(1), alpha(2)	2	0				
K+	OH-	beta(0)	147.00940705996	-0.59063893403091	0	0.00078787849058873	0	0
K+	OH-	beta(1)	-2151.130770341	12.657469805761	0	-0.017131182753022	0	0
K+	OH-	Cphi	-22.315984605208	0.13692712105358	0	-0.00020221458776836	0	0
K+	OH-	alpha(1), alpha(2)	2	0				
K+	SO4-2	beta(0)	-14114.520235733	604.5925786277	-111.05626428528	0.29099890961573	-0.00012610398328222	0
K+	SO4-2	beta(1)	25616.79189368	-1322.5700475074	252.60626183174	-0.80171327199471	0.0004186181651332	0
K+	SO4-2	Cphi	9686.0875025558	-418.49135389981	76.990124012268	-0.20302803127067	0.000088625084082025	0
K+	SO4-2	alpha(1), alpha(2)	2	0				
Mg+2	Cl-	beta(0)	-9.5949075987732	0.52058075085694	0	-0.00045632571158819	0	0
Mg+2	Cl-	beta(1)	1239.2880942931	-7.3631696542185	0	0.016394622815563	0	0
Mg+2	Cl-	Cphi	12.528229322268	-0.045346523422936	0	0.000028564736424319	0	0
Mg+2	Cl-	alpha(1), alpha(2)	2	0				
Mg+2	HSO4-	beta(0)	-231093.45360515	4168.9585266703	-654.03512875098	0.61027675302183	0	13434138.420831
Mg+2	HSO4-	beta(1)	0	1.7289792050033	0	0	0	0
Mg+2	HSO4-	Cphi	-55992.114162006	1096.9039631968	-174.81198244032	0.17956232737988	0	2964964.3394071
Mg+2	HSO4-	alpha(1), alpha(2)	2	0				

Tab. 2 (continued)

			a	b	c	d	e	f
Mg+2	SO4-2	beta(0)	165423.9906188	-3907.3147032293	658.46229851464	-1.1598500501533	0.00038270739671658	-7748191.3861327
Mg+2	SO4-2	beta(1)	55777.546009983	-1872.4550736665	340.94273642432	-0.92294789945276	0.00047034934295508	-1819568.1965241
Mg+2	SO4-2	beta(2)	0	13318.126201215	-3193.0895050815	21.925295748391	-0.019118021865416	0
Mg+2	SO4-2	Cphi	2488.0005592639	-73.329119045042	12.705371182873	-0.024264178	0.0000069398165325636	-67851.92125
Mg+2	SO4-2	alpha(1), alpha(2)	1.4	12				
Na+	Cl-	beta(0)	-3062.3742486018	132.26053520957	-24.400201527452	0.066632203018823	-0.000031024626856696	0
Na+	Cl-	beta(1)	-6499.63324794035	295.616553490889	-55.0111433640026	0.155286132298996	-0.0000720751331288712	0
Na+	Cl-	Cphi	-5520.47046244513	138.107436887365	-23.5679175416441	0.0448064311022912	-0.0000159669079559805	244503.571832341
Na+	Cl-	alpha(1), alpha(2)	2	0				
Na+	HSO4-	beta(0)	-447.90677731674	26.213145709303	-5.0006267881412	0.015156973239521	-0.0000071150145889711	-10.641894979855
Na+	HSO4-	beta(1)	282.41816236695	-21.918105273919	3.1531865163269	0.018747217872392	-0.000028837959348127	7.2454235949245
Na+	HSO4-	Cphi	94.829903241325	-5.503962125203	1.0586866346744	-0.0033388376450779	0.0000016148627458055	1.862581604426
Na+	HSO4-	alpha(1), alpha(2)	2	0				
Na+	OH-	beta(0)	-98.888405195742	0.74845113296049	0	-0.0010478515797703	0	0
Na+	OH-	beta(1)	-206.11199903783	1.2022295299777	0	-0.0012958058812917	0	0
Na+	OH-	Cphi	17.300056299236	-0.091131605628721	0	0.00011826675205965	0	0
Na+	OH-	alpha(1), alpha(2)	2	0				
Na+	SO4-2	beta(0)	1052.0403467436	-44.400069456973	7.8553275217993	-0.012964613626797	0	0
Na+	SO4-2	beta(1)	-50431.463443382	1702.9905586626	-291.10699873715	0.42220582235853	0	0
Na+	SO4-2	Cphi	-494.28155511456	18.045079042636	-3.1202844717061	0.004681676697336	0	0
Na+	SO4-2	alpha(1), alpha(2)	2	0				

\* The interaction of  $\text{Ca}^{2+}$  and  $\text{OH}^-$  needs a beta(2) value to properly describe the effect of weak association. According to literature [HAR/MOL1984], alpha(1)=2.0 and alpha(2) should be set to 12.0 for such cases. The first parametrisation of the Pitzer model for THEREDA was performed with the program ChemSage/ChemApp, which in the beginning did not allow the definition of a designated value for alpha(2). The source code of the program isn't accessible. But it turned out that for any case where a value for beta(2)  $\neq$  0 is entered for electrolytes with one monovalent and one higher valent ion, alpha(2) is automatically set to 50. Hence, the parametrisation of the present model was based unintentionally on an alpha(2) value of 50 for the present interaction between  $\text{Ca}^{2+}$  and  $\text{OH}^-$ . Since all experimental data are represented well within their experimental error, this (albeit unusual) alpha(2) value of 50 was adopted into the database.

Tab. 3: Temperature coefficients of the equation for the Pitzer parameter (theta).

$$P = \frac{a}{T} + b + c \cdot \ln(T) + d \cdot T + e \cdot T^2 + \frac{f}{T^2}$$

theta		a	b	c	d	e	f
Ca+2	H+	0	0.096861568224187	0	0	0	0
Cl-	HSO4-	0	0	0	0	0	0
Cl-	SO4-2	614.5226089362	-4.0149983991821	0	0.0066204233736244	0	0
K+	Ca+2	0	0.11559860965783	0	0	0	0
K+	H+	-55.875359263937	0.20278430500932	0	0	0	0
K+	Mg+2	-1048.5973881773	5.8786678886283	0	-0.0079210297311925	0	0
Mg+2	Ca+2	-4785.6280582116	225.36273870948	-42.263061386734	0.12329171808287	-0.000059523467917494	0
Mg+2	H+	0	0.51653862168501	0	-0.0031309680558061	0.0000058285013290036	0
Na+	Ca+2	2267.2117127993	-81.053952529918	14.014772007938	-0.021273515304588	0	0
Na+	H+	-4.0542575885501	0.048135767274039	0	0	0	0
Na+	K+	0	-0.012043927235552	0	1.4781672211197E-07	0	0
Na+	Mg+2	0	-0.063343456551807	0	0.00044723332094534	0	0
OH-	Cl-	-49.361345504841	0.11048570304889	0	0	0	0
OH-	SO4-2	0	-0.33575218581995	0.14531158458115	-0.0022722938962054	0.0000019538423356786	0
SO4-2	HSO4-	121059.80972999	-2844.522811955	478.64841878646	-0.83397701136569	0.00027042821215948	-5704023.4169222

Tab. 4: Temperature coefficients of the equation for the Pitzer parameter (psi).

$$P = \frac{a}{T} + b + c \cdot \ln(T) + d \cdot T + e \cdot T^2 + \frac{f}{T^2}$$

psi			a	b	c	d	e	f
Ca+2	Cl-	HSO4-	0	175.9718762403	-40.770364736304	0.24044838306573	-0.00017294791989897	0
Ca+2	Cl-	OH-	98.197927897047	-0.82029144903482	0	0.0015196827300499	0	0
Ca+2	Cl-	SO4-2	0	-0.017920500330748	0	0	0	0
Ca+2	H+	Cl-	19.81649946479	-0.20840514246196	0.01716608551326	0.00010808358001082	0	0
Ca+2	H+	HSO4-	0	0	0	0	0	0
Ca+2	H+	SO4-2	0	0	0	0	0	0
Ca+2	SO4-2	HSO4-	-1756.3687257201	45.111773528174	-7.2842510000601	0.0070015551265861	0	0
K+	Ca+2	Cl-	-27.076725039389	0.047627324914306	0	0	0	0
K+	Cl-	OH-	-1.7041006193998	-0.0035398452300198	0	2.02194E-05	0	0
K+	Cl-	SO4-2	-206.37961777617	1.2883646581274	0	-0.0019995439509291	0	0
K+	H+	Cl-	43.641634505983	-0.80328100366829	0.11186779758254	0.000021245520115461	0	0
K+	H+	HSO4-	0	-38.556260568886	8.9118197895243	-0.052680816405075	0.000038989631006074	0
K+	H+	SO4-2	-40.466204101269	0.1298754999098	0	0	0	0
K+	Mg+2	Cl-	332.1117055746	-2.4074372638162	0	0.0053773109904384	-0.0000037316131192495	0
K+	Mg+2	SO4-2	5156.2969511095	-200.04065187323	35.790366227674	-0.079512841289314	0.000027966251728907	0
K+	SO4-2	OH-	-42.09030770341	0.13144059402249	0	0	0	0
Mg+2	Ca+2	Cl-	-1.2470933044681	-16.410481508209	3.8980831378916	-0.025664432256901	0.000020755538998136	0
Mg+2	Ca+2	SO4-2	-2574.0685192579	54.255844305731	-8.0094078826147	0	0	0
Mg+2	Cl-	SO4-2	-669.97194202899	5.835016300439	0	-0.016474198701064	0.000014847701425221	0
Mg+2	H+	Cl-	-1357.291354862	61.244574321968	-11.309231470323	0.029270572012749	-0.000011173505755006	-33.683663900415
Mg+2	H+	HSO4-	0	-0.01779978591617	0	0	0	0
Mg+2	H+	SO4-2	0	0	0	0	0	0
Na+	Ca+2	Cl-	-6187.9848457514	302.35739705815	-57.161708609056	0.1738529135847	-0.000087225483432558	0
Na+	Ca+2	OH-	0	5086.7271220654	-1196.0108422476	7.5376900425161	-0.005843478	0
Na+	Ca+2	SO4-2	541.22316435143	-29.266691709664	5.6455312394011	-0.018943553671297	0.00001022002329665	0



Tab 4 (continued)

psi			a	b	c	d	e	f
Na+	Cl-	OH-	0	-3.61342282638764	0.828412891695231	-0.00473162879186962	0.00000337394750135306	0
Na+	Cl-	SO4-2	-128.330056527753	0.861364516567442	0	-0.00144069567262012	0	0
Na+	H+	Cl-	3.59304603523964	-0.0145621583979794	0	0	0	0
Na+	H+	HSO4-	0	-0.0146327340188827	0	0	0	0
Na+	H+	SO4-2	2.47898831439052	0.00476198151422214	0	0	0	0
Na+	HSO4-	SO4-2	19.8971943953335	-0.103379626676288	0	0.000140453143303867	0	0
Na+	K+	Cl-	0	-0.0079019352865476	0	0.0000204660638523062	0	0
Na+	K+	OH-	-184.02481604426	1.09189586998617	0	-0.00160450254014072	0	0
Na+	K+	SO4-2	0	-0.115537956088761	0	0.000353976442600277	0	0
Na+	Mg+2	Cl-	0	-2.67633662036202	0.618873156654038	-0.00367854306693126	0.00000264366820374045	0
Na+	Mg+2	SO4-2	-73.684333778339	0.464811810211077	0	-0.000780389614047748	0	0
Na+	SO4-2	OH-	-2.55446774430212	-0.046979066690721	0	0.000147735612003127	0	0