

Appendix B (part 1/2) : Data used for establish $\Delta H^\circ_{f, 298.15K}$ estimation model for hydrated sulfates. (formula and all values are per one SO_4).

Mineral	Formula	(I)	(II)	(III)	(IV)	(V)	(VI)
		$\Delta H^\circ_{f,298.15K}$ (kJ.mol ⁻¹)	ΔH°_{hyd} (kJ.mol ⁻¹)	n H ₂ O	ΔH°_{diss} (kJ.mol ⁻¹)	ΔH°_f calc (kJ.mol ⁻¹)	Error (%)
Bassanite	KCu _{0.5} (SO ₄) · 0.25H ₂ O	-1180.70 ¹	-2.42	0.25	-24.19	-1181.93	-0.10
	CaSO ₄ · 0.5H ₂ O	-1576.74 ¹	-4.55	0.5	-18.23	-1584.40	-0.49
Bassanite	CaSO ₄ · 0.5H ₂ O	-1574.65 ¹	-6.90	0.5	-18.23	-1584.40	-0.62
Zr-Sulfate	Zr _{0.5} (SO ₄) · 0.5H ₂ O	-1276.95 ¹	-21.45	0.5	-104.69	-1276.90	0.00
Kieserite	MgSO ₄ · H ₂ O	-1602.10 ¹	-23.29	1	-91.44	-1602.15	0.00
Kieserite	MgSO ₄ · H ₂ O	-1612.40 ⁴	-33.59	1	-91.44	-1598.08	0.89
Cobaltkieserite	NaMn _{0.5} (SO ₄) · H ₂ O	-1540.15 ¹	-0.89	1	-14.69	-1542.51	-0.15
	KMg _{0.5} (SO ₄) · H ₂ O	-1675.70 ¹	-4.44	1	-17.59	-1675.27	0.03
	KMn _{0.5} (SO ₄) · H ₂ O	-1559.40 ¹	-11.34	1	-17.69	-1552.09	0.47
	KZn _{0.5} (SO ₄) · H ₂ O	-1518.80 ¹	-7.74	1	-20.99	-1515.96	0.19
	KCu _{0.5} (SO ₄) · H ₂ O	-1413.35 ¹	-14.64	1	-24.19	-1404.45	0.63
	KCu _{0.5} (SO ₄) · H ₂ O	-1413.35 ¹	-7.54	1	-24.19	-1411.55	0.13
	NaZn _{0.5} (SO ₄) · H ₂ O	-1507.10 ¹	-4.19	1	-17.34	-1506.85	0.02
	ZnSO ₄ · H ₂ O	-1304.49 ¹	-27.78	1	-79.94	-1297.04	0.57
	CdSO ₄ · H ₂ O	-1239.55 ¹	-12.36	1	-51.96	-1240.20	-0.05
	CdSO ₄ · H ₂ O	-1240.05 ³	-12.57	1	-51.67	-1240.41	-0.03
	CuSO ₄ · H ₂ O	-1085.83 ¹	-20.56	1	-73.08	-1083.80	0.19
	NiSO ₄ · H ₂ O	-1190.89 ³	-23.45	1	-89.81	-1190.35	0.05
	CoSO ₄ · H ₂ O	-1201.53 ¹	-17.67	1	-77.59	-1203.57	-0.17
	FeSO ₄ · H ₂ O	-1243.69 ¹	-21.38	1	-72.04	-1240.57	0.25
	FeSO ₄ · H ₂ O	-1244.30 ²	-21.99	1	-72.04	-1240.57	0.30
	FeSO ₄ · H ₂ O	-1244.82 ³	-21.86	1	-71.39	-1241.05	0.30
	MnSO ₄ · H ₂ O	-1376.50 ¹	-17.34	1	-64.89	-1375.55	0.07
	MnSO ₄ · H ₂ O	-1378.13 ³	-17.72	1	-63.64	-1376.47	0.12
	UO ₂ SO ₄ · H ₂ O	-2146.40 ¹	-7.39	1	-83.24	-2160.20	-0.64
	BeSO ₄ · H ₂ O	-1523.80 ¹	-24.69	1	-86.94	-1521.27	0.17
Li ₂ SO ₄ · H ₂ O	-1735.50 ¹	-5.10	1	-29.85	-1737.62	-0.12	
Li ₂ SO ₄ · H ₂ O	-1735.05 ³	-4.32	1	-29.85	-1737.95	-0.17	
K _{0.5} Al _{0.5} (SO ₄) · 1.5H ₂ O	-1690.55 ⁷	-14.59	1.5	-69.49	-1696.04	-0.32	
Al _{2/3} (SO ₄) · 2H ₂ O	-1770.57 ¹	-35.81	2	-121.33	-1773.82	-0.18	
Al _{2/3} (SO ₄) · 2H ₂ O	-1771.76 ³	-36.23	2	-121.33	-1773.82	-0.12	
MgSO ₄ · 2H ₂ O	-1896.20 ¹	-23.49	2	-91.44	-1901.97	-0.30	
MgSO ₄ · 2H ₂ O	-1894.90 ⁴	-22.19	2	-91.44	-1897.90	-0.16	
CaSO ₄ · 2H ₂ O	-2022.63 ¹	-0.71	2	-18.23	-2027.16	-0.22	
CaSO ₄ · 2H ₂ O	-2023.00 ²	-0.79	2	-18.23	-2027.45	-0.22	
CaSO ₄ · 2H ₂ O	-2023.82 ³	-0.86	2	-18.23	-2028.20	-0.22	
KMg _{0.5} (SO ₄) · 2H ₂ O	-1973.80 ¹	-8.64	2	-17.59	-1970.19	0.18	
KMg _{0.5} (SO ₄) · 2H ₂ O	-1975.50 ³	-10.33	2	-17.59	-1970.19	0.27	
KMn _{0.5} (SO ₄) · 2H ₂ O	-1852.70 ¹	-10.74	2	-17.69	-1847.02	0.31	
NaZn _{0.5} (SO ₄) · 2H ₂ O	-1796.00 ¹	0.81	2	-17.34	-1801.76	-0.32	
Zr _{0.5} (SO ₄) · 2H ₂ O	-1727.15 ¹	-30.79	2	-104.69	-1729.97	-0.16	
BeSO ₄ · 2H ₂ O	-1823.14 ¹	-30.13	2	-86.94	-1820.79	0.13	
BeSO ₄ · 2H ₂ O	-1824.40 ³	-30.25	2	-85.80	-1821.56	0.16	
UO ₂ SO ₄ · 2.5H ₂ O	-2607.10 ¹	-27.24	2.5	-83.24	-2608.44	-0.05	
UO ₂ SO ₄ · 2.5H ₂ O	-2607.50 ⁵	-27.64	2.5	-83.24	-2608.48	-0.04	
Fe _{2/3} (SO ₄) · 2.58H ₂ O	-1638.73 ⁶	-18.98	2.58	-82.11	-1648.95	-0.62	
Sm _{2/3} (SO ₄) · 8/3H ₂ O	-2110.27 ¹	-26.82	2.67	-70.71	-2108.11	0.10	
CdSO ₄ · 8/3H ₂ O	-1729.40 ¹	-12.37	2.67	-51.96	-1735.92	-0.38	
CdSO ₄ · 8/3H ₂ O	-1730.11 ³	-12.79	2.67	-51.67	-1736.11	-0.35	
KMg _{0.5} (SO ₄) · 3H ₂ O	-2269.80 ¹	-10.73	3	-17.59	-2264.81	0.22	
KMg _{0.5} (SO ₄) · 3H ₂ O	-2270.73 ³	-11.66	3	-17.59	-2264.81	0.26	
KZn _{0.5} (SO ₄) · 3H ₂ O	-2117.10 ¹	-18.23	3	-20.99	-2105.88	0.53	

Mineral	Formula	(I) $\Delta H_{f,298.5K}^{\circ}$ (kJ.mol ⁻¹)	(II) ΔH_{hyd}° (kJ.mol ⁻¹)	(III) n H ₂ O	(IV) ΔH_{diss}° (kJ.mol ⁻¹)	(V) ΔH_f° calc (kJ.mol ⁻¹)	(VI) Error (%)
Banattite	CuSO ₄ · 3H ₂ O	-1684.31 ¹	-31.23	3	-73.08	-1679.59	0.28
Coquimbite	Fe _{2/3} (SO ₄) · 3H ₂ O	-1765.13 ⁶	-22.92	3	-82.11	-1772.84	-0.44
	La _{2/3} (SO ₄) · 3 H ₂ O	-2216.00 ¹	-20.52	3	-66.97	-2219.71	-0.17
	UO ₂ SO ₄ · 3H ₂ O	-2754.30 ¹	-27.48	3	-83.24	-2757.14	-0.10
	UO ₂ SO ₄ · 3H ₂ O	-2755.29 ⁵	-28.47	3	-83.24	-2757.18	-0.07
	UO ₂ SO ₄ · 3.5H ₂ O	-2900.80 ¹	-27.03	3.5	-83.24	-2905.65	-0.17
	UO ₂ SO ₄ · 3.5H ₂ O	-2901.60 ⁵	-27.83	3.5	-83.24	-2905.69	-0.14
Starkeyite	MgSO ₄ · 4H ₂ O	-2496.60 ¹	-36.08	4	-91.44	-2497.20	-0.02
Starkeyite	MgSO ₄ · 4H ₂ O	-2497.30 ³	-40.85	4	-91.44	-2493.13	0.17
	NiSO ₄ · 4H ₂ O	-2104.10 ¹	-55.57	4	-90.43	-2084.79	0.92
Rozenite	FeSO ₄ · 4H ₂ O	-2129.20 ¹	-25.18	4	-72.04	-2132.72	-0.17
	MnSO ₄ · 4H ₂ O	-2258.10 ¹	-17.23	4	-64.89	-2266.63	-0.38
	MnSO ₄ · 4H ₂ O	-2258.74 ³	-16.62	4	-63.64	-2267.36	-0.38
	BeSO ₄ · 4H ₂ O	-2423.75 ¹	-42.93	4	-86.94	-2415.64	0.33
	BeSO ₄ · 4H ₂ O	-2425.75 ³	-43.79	4	-85.80	-2416.32	0.39
Chalcanthite	CuSO ₄ · 5H ₂ O	-2279.62 ¹	-38.73	5	-73.08	-2272.21	0.33
Chalcanthite	CuSO ₄ · 5H ₂ O	-2279.70 ²	-38.77	5	-73.04	-2272.23	0.33
Chalcanthite	CuSO ₄ · 5H ₂ O	-2280.47 ³	-40.57	5	-74.07	-2271.65	0.39
Jokokuite	MnSO ₄ · 5H ₂ O	-2553.10 ¹	-18.32	5	-64.89	-2562.47	-0.37
	Al _{2/3} (SO ₄) · 6H ₂ O	-2959.63 ¹	-49.25	6	-121.33	-2966.26	-0.22
	Al _{2/3} (SO ₄) · 6H ₂ O	-2961.60 ³	-50.45	6	-121.33	-2966.26	-0.16
Hexahydrate	MgSO ₄ · 6H ₂ O	-3087.00 ¹	-38.67	6	-91.44	-3090.19	-0.10
Hexahydrate	MgSO ₄ · 6H ₂ O	-3088.06 ³	-43.80	6	-91.44	-3086.12	0.06
Hexahydrate	MgSO ₄ · 6H ₂ O	-3088.10 ⁴	-39.77	6	-91.44	-3086.12	0.06
Alum-K	K _{0.5} Al _{0.5} (SO ₄) · 6H ₂ O	-3030.90 ¹	-32.37	6	-69.49	-3030.08	0.03
Alum-K	K _{0.5} Al _{0.5} (SO ₄) · 6H ₂ O	-3030.90 ⁷	-32.55	6	-69.49	-3027.67	0.03
Alum-K	K _{0.5} Al _{0.5} (SO ₄) · 6H ₂ O	-3033.00 ³	-33.75	6	-69.49	-3030.80	0.07
Tschermigite	(NH ₄) _{0.5} Al _{0.5} (SO ₄) · 6H ₂ O	-2971.19 ¹	-31.65	6	-69.09	-2970.90	0.01
Tschermigite	(NH ₄) _{0.5} Al _{0.5} (SO ₄) · 6H ₂ O	-2973.17 ³	-32.83	6	-68.28	-2971.33	0.06
Bianchite	ZnSO ₄ · 6 H ₂ O	-2779.65 ³	-35.76	6	-82.28	-2781.45	-0.06
Retgersite	NiSO ₄ · 6H ₂ O	-2682.82 ¹	-46.48	6	-90.43	-2677.72	0.19
Retgersite	NiSO ₄ · 6H ₂ O	-2683.40 ²	-46.77	6	-90.14	-2677.88	0.21
Retgersite	NiSO ₄ · 6H ₂ O	-2684.41 ³	-47.45	6	-89.81	-2678.05	0.24
	CoSO ₄ · 6H ₂ O	-2683.60 ¹	-31.87	6	-79.24	-2687.86	-0.16
	CoSO ₄ · 6H ₂ O	-2685.29 ³	-31.91	6	-77.59	-2688.74	-0.13
Epsomite	MgSO ₄ · 7H ₂ O	-3388.71 ¹	-46.47	7	-91.44	-3386.25	0.07
Epsomite	MgSO ₄ · 7H ₂ O	-3388.70 ²	-46.46	7	-91.44	-3386.25	0.07
Epsomite	MgSO ₄ · 7H ₂ O	-3390.05 ³	-51.88	7	-91.44	-3382.18	0.23
Epsomite	MgSO ₄ · 7H ₂ O	-3387.70 ⁴	-45.46	7	-91.44	-3382.18	0.16
Goslarite	ZnSO ₄ · 7 H ₂ O	-3077.75 ¹	-37.61	7	-79.94	-3078.47	-0.02
Goslarite	ZnSO ₄ · 7 H ₂ O	-3077.50 ²	-40.06	7	-82.64	-3077.10	0.01
Goslarite	ZnSO ₄ · 7 H ₂ O	-3079.14 ³	-41.34	7	-82.28	-3077.29	0.06
Morenosite	NiSO ₄ · 7H ₂ O	-2976.33 ¹	-46.08	7	-90.43	-2973.76	0.09
Morenosite	NiSO ₄ · 7H ₂ O	-2976.50 ²	-45.96	7	-90.14	-2973.91	0.09
Morenosite	NiSO ₄ · 7H ₂ O	-2978.11 ³	-47.24	7	-89.81	-2974.07	0.14
Bieberite	CoSO ₄ · 7H ₂ O	-2979.93 ¹	-34.29	7	-79.24	-2983.63	-0.12
Bieberite	CoSO ₄ · 7H ₂ O	-2981.59 ³	-34.30	7	-77.59	-2984.46	-0.10
Melanterite	FeSO ₄ · 7H ₂ O	-3014.57 ¹	-28.83	7	-72.04	-3020.17	-0.19
Melanterite	FeSO ₄ · 7H ₂ O	-3014.30 ²	-28.56	7	-72.04	-3020.17	-0.19
Melanterite	FeSO ₄ · 7H ₂ O	-3016.51 ³	-30.12	7	-71.39	-3020.50	-0.13
Mallardite	MnSO ₄ · 7H ₂ O	-3139.30 ¹	-16.71	7	-64.89	-3153.49	-0.45
Mallardite	MnSO ₄ · 7H ₂ O	-3140.90 ³	-17.06	7	-63.64	-3154.13	-0.42
Mirabilite	Na ₂ SO ₄ · 10H ₂ O	-4327.26 ¹	-1.13	10	-2.86	-4326.47	0.02
Mirabilite	Na ₂ SO ₄ · 10H ₂ O	-4327.30 ²	-0.45	10	-2.86	-4327.19	0.00
Mirabilite	Na ₂ SO ₄ · 10H ₂ O	-4330.83 ³	-2.98	10	-2.86	-4328.19	0.06

Footnote added at the end of Appendix B

Colonne (I) : experimental values of $\Delta H^\circ_{f,298.15K}$ (for one SO_4) for hydrous sulfates from references (in exponent): 1- Wagman et al. (1982); 2- Robie and Hemingway (1995); 3- Naumov et al. (1971); 4- Grevel and Majzlan (2011); 5- Grenthe et al. (1992); 6- Ackermann et al. (2009); 7- Barin (1985)

Column (II): ΔH°_{hyd} . Enthalpy of hydration of hydrous sulfate per one SO_4 ;

Column (III): number of moles of hydration water (per one SO_4)

Column (IV): Enthalpy of dissolution (per one SO_4) of anhydrous analogue;

Column (V): ΔH°_{ox} . Predicted enthalpy of formation of hydrous sulfate (Eqn. (26));

Column (VI): % error between predicted enthalpy of formation (Column V) and experimental enthalpy of formation (Column I) for hydrous sulfates