

Appendix A (part 1/2): Data used to establish $\Delta H^\circ_{f, 298.15K}$ estimation model of anhydrous sulfates.

Mineral/Compound	Formula	(I) $\Delta H^\circ_{f, 298.15K}$ (kJ.mol ⁻¹)	(II) $\Delta H^\circ_{f, ox}$ (kJ.mol ⁻¹)	(III) $\Delta H^\circ_{f, (es, aq)}$ (kJ.mol ⁻¹)	(IV) error (%)	(V) $\Delta H^\circ_{f, (es, cr)}$ (kJ.mol ⁻¹)	(VI) error (%)
Thenardite	Na ₂ SO ₄	-1387.08 ¹	-517.77	-1395.95	-0.64	-1380.65	0.46
		-1387.80 ²	-518.49	-1395.95	-0.59	-1380.65	0.52
		-1388.80 ³	-519.49	-1395.95	-0.52	-1380.65	0.59
Arcanite	K ₂ SO ₄	-1437.79 ¹	-620.08	-1437.41	0.03	-1418.22	1.36
		-1437.70 ²	-619.99	-1437.41	0.02	-1418.22	1.35
		-1433.69 ⁷	-615.98	-1437.41	-0.26	-1418.22	1.08
		-1438.65 ³	-620.94	-1437.41	0.09	-1418.22	1.42
Mascagnite	(NH ₄) ₂ SO ₄	-1180.85 ¹	-295.64	-1127.35	4.53	-1187.59	-0.57
		-1182.70 ²	-297.49	-1127.35	4.68	-1187.59	-0.41
		-1180.80 ³	-295.59	-1127.35	4.53	-1187.59	-0.58
Anhydrite	CaSO ₄	-1434.11 ¹	-344.5	-1420.85	0.92	-1429.56	0.32
		-1425.24 ¹	-335.63	-1420.85	0.31	-1429.56	-0.30
		-1420.80 ¹	-331.19	-1420.85	0.00	-1429.56	-0.62
		-1434.40 ²	-344.79	-1420.85	0.94	-1429.56	0.34
		-1435.15 ³	-345.54	-1420.85	1.00	-1429.56	0.39
Baryte	BaSO ₄	-1473.20 ¹	-470.59	-1428.52	3.03	-1468.34	0.33
		-1473.60 ²	-470.99	-1428.52	3.06	-1468.34	0.36
		-1458.35 ³	-455.74	-1428.52	2.05	-1468.34	-0.69
Mg-sulfate	MgSO ₄	-1284.90 ¹	-228.79	-1334.76	-3.88	-1282.00	0.23
		-1284.90 ²	-228.79	-1334.76	-3.88	-1282.00	0.23
		-1280.83 ³	-224.72	-1334.76	-4.21	-1282.00	-0.09
Mn-sulfate	MnSO ₄	-1065.25 ¹	-225.54	-1081.48	-1.52	-1058.89	0.60
		-1065.70 ²	-225.99	-1081.48	-1.48	-1058.89	0.64
		-1066.50 ³	-226.79	-1081.48	-1.40	-1058.89	0.71
Anglesite	PbSO ₄	-919.94 ¹	-246.43	-846.60	7.97	-918.82	0.12
		-920.00 ²	-246.49	-846.60	7.98	-918.82	0.13
		-919.92 ³	-246.41	-846.60	7.97	-918.82	0.12
Zincosite	ZnSO ₄	-982.80 ¹	-177.79	-1006.30	-2.39	-976.39	0.65
		-980.10 ²	-175.09	-1006.30	-2.67	-976.39	0.38
		-980.46 ³	-175.45	-1006.30	-2.64	-976.39	0.42
Cd-sulfate	CdSO ₄	-933.28 ¹	-220.42	-932.32	0.10	-925.76	0.81
		-933.57 ³	-220.71	-932.32	0.13	-925.76	0.84
Chalcocyanite	CuSO ₄	-771.36 ¹	-160.75	-782.34	-1.42	-772.23	-0.11
		-771.40 ²	-160.79	-782.34	-1.42	-772.23	-0.11
		-770.37 ³	-159.76	-782.34	-1.55	-772.23	-0.24
	SrSO ₄	-1453.10 ¹	-407.29	-1441.03	0.83	-1453.08	0.00
Mikasaite	Fe ₂ (SO ₄) ₃	-2581.50 ¹	-130.59	-2626.46	-1.74	-2577.55	0.15
		-2581.90 ²	-130.72	-2626.46	-1.73	-2577.55	0.17
		-2583.67 ³	-131.31	-2626.46	-1.66	-2577.55	0.24
Millosevichite	Al ₂ (SO ₄) ₃	-3440.84 ¹	-133.87	-3633.74	-5.61	-3438.49	0.07
		-3441.80 ²	-134.19	-3633.74	-5.58	-3438.49	0.10
		-3443.15 ³	-134.64	-3633.74	-5.54	-3438.49	0.14
Godovikovite	NH ₄ Al(SO ₄) ₂	-2352.20 ¹	-194.99	-2386.04	-1.44	-2334.20	0.77
		-2353.82 ³	-195.8	-2386.04	-1.37	-2334.20	0.83
Yavapaiite	KFe(SO ₄) ₂	-2042.80 ⁶	-269.54	-2091.20	-2.37	-2056.79	-0.68
Steklite	KAl(SO ₄) ₂	-2470.20 ¹	-270.86	-2588.27	-4.78	-2486.78	-0.67
		-2470.90 ²	-271.25	-2588.27	-4.75	-2486.78	-0.64
		-2471.64 ³	-271.58	-2588.27	-4.72	-2486.78	-0.61
Zn-glauberite	Na ₂ Zn(SO ₄) ₂	-2418.00 ¹	-371.84	-2456.48	-1.59	-2413.70	0.18
Glauberite	Na ₂ Ca(SO ₄) ₂	-2829.20 ¹	-435.14	-2849.37	-0.71	-2838.77	-0.34
Mn-glauberite	Na ₂ Mn(SO ₄) ₂	-2490.70 ¹	-390.84	-2524.91	-1.37	-2488.23	0.10
Mg-glauberite	Na ₂ Mg(SO ₄) ₂	-2691.10 ¹	-382.84	-2772.04	-3.01	-2710.22	-0.71

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Mineral/Compound	Formula	(I) $\Delta H^\circ_{f, 298.15K}$ (kJ.mol ⁻¹)	(II) $\Delta H^\circ_{f, ox}$ (kJ.mol ⁻¹)	(III) $\Delta H^\circ_{f (es, aq)}$ (kJ.mol ⁻¹)	(IV) error (%)	(V) $\Delta H^\circ_{f (es, cr)}$ (kJ.mol ⁻¹)	(VI) error (%)
	Na ₂ Sr(SO ₄) ₂	-2830.10 ¹	-457.49	-2858.89	-1.02	-2834.39	-0.15
	Na ₂ Ba(SO ₄) ₂	-2853.90 ¹	-490.99	-2841.26	0.44	-2856.59	-0.09
	(NH ₄) ₂ Sr(SO ₄) ₂	-2639.30 ¹	-354.14	-2593.90	1.72	-2634.80	0.17
	(NH ₄) ₂ Cu(SO ₄) ₂	-2054.30 ¹	-279.24	-1921.43	6.47	-1983.28	3.46
	(NH ₄) ₂ Zn(SO ₄) ₂	-2201.60 ¹	-255.69	-2140.46	2.78	-2185.81	0.72
	K ₂ Sr(SO ₄) ₂	-2887.40 ¹	-511.94	-2915.86	-0.99	-2886.82	0.02
	K ₂ Ba(SO ₄) ₂	-2907.90 ¹	-543.79	-2898.23	0.33	-2909.03	-0.04
	K ₂ Na ₂ (SO ₄) ₂	-2821.30 ¹	-567.14	-2848.88	-0.98	-2813.73	0.27
Palmierite	K ₂ Pb(SO ₄) ₂	-2379.90 ¹	-444.34	-2358.45	0.90	-2396.24	-0.69
	K ₂ Zn(SO ₄) ₂	-2434.30 ¹	-405.79	-2513.45	-3.25	-2466.13	-1.31
Cyanochroite anh.	K ₂ Cu(SO ₄) ₂	-2209.60 ¹	-397.74	-2294.41	-3.84	-2263.60	-1.79
	K ₂ Mn(SO ₄) ₂	-2508.30 ¹	-425.44	-2581.88	-2.93	-2540.66	-1.29
Leonite anh.	K ₂ Mg(SO ₄) ₂	-2754.70 ¹	-440.44	-2829.01	-2.70	-2762.66	-0.29
Langbeinite	K ₂ Mg ₂ (SO ₄) ₃	-4071.00 ²	-380.36	-4182.72	-2.74	-4065.47	0.14
		-4073.00 ³	-381.02	-4182.72	-2.69	-4065.47	0.18
Zn-langbeinite	K ₂ Zn ₂ (SO ₄) ₃	-3406.85 ⁴	-326.37	-3543.00	-4.00	-3466.36	-1.75
Cd-langbeinite	K ₂ Cd ₂ (SO ₄) ₃	-3305.52 ⁴	-354.03	-3390.99	-2.59	-3355.88	-1.52
Cd-effremovite	(NH ₄) ₂ Cd ₂ (SO ₄) ₃	-3031.74 ⁵	-240.27	-2997.03	1.14	-3059.00	-0.90
Mn-effremovite	(NH ₄) ₂ Mn ₂ (SO ₄) ₃	-3250.16 ⁵	-228.51	-3290.39	-1.24	-3323.86	-2.27
Vanthoffite	Na ₆ Mg(SO ₄) ₄	-5461.81 ³	-449.44	-5584.62	-2.25	-5495.31	-0.61
Eugsterite anh.	Na ₄ Ca(SO ₄) ₃	-4230.00 ¹	-467.26	-4256.18	-0.62	-4228.94	0.02
	Na ₄ Sr(SO ₄) ₃	-4209.10 ¹	-474.89	-4262.14	-1.26	-4221.93	-0.30
	Na ₄ Ba(SO ₄) ₃	-4240.10 ¹	-499.62	-4242.81	-0.06	-4239.77	0.01
	K ₄ Sr(SO ₄) ₃	-4323.30 ¹	-547.36	-4365.74	-0.98	-4316.89	0.15
	K ₄ Ba(SO ₄) ₃	-4342.20 ¹	-568.06	-4346.41	-0.10	-4334.74	0.17
	Na ₄ K ₂ (SO ₄) ₃	-4204.50 ¹	-549.39	-4250.00	-1.08	-4199.33	0.12
	K ₄ Na ₂ (SO ₄) ₃	-4263.90 ¹	-586.39	-4291.46	-0.65	-4236.91	0.63
	Na ₂ K ₆ (SO ₄) ₄	-5709.24 ¹	-596.70	-5731.46	-0.39	-5657.60	0.90
Mercallite	KHSO ₄	-1160.60 ¹	-381.58	-1178.64	-1.55	-1156.16	0.38
Na-mercallite	NaHSO ₄	-1125.50 ¹	-320.68	-1150.16	-2.19	-1129.94	-0.39

Footnote added at the end of Appendix A:

Anh.: Anhydrous form

Column (I): enthalpy of formation of anhydrous salt from reference (in exponent) 1 - Wagman et al. (1982); 2 - Robie and Hemingway (1995); 3 - Naumov et al. (1971); 4 - Zhou et al. (2001b); 5 - Zhou et al. (2001a); 6 - Forray et al. (2005); 7 - Barin (1985)

Column (II): enthalpy of formation of anhydrous salt from constituent oxides per one mole of SO₄;Column (III): predicted enthalpy of formation of anhydrous salt with parameters $\Delta_H O^\circ M_i^{Z_i+} (aq)$;

Column (IV): % error between predicted enthalpy of formation (Column III) and experimental enthalpy of formation (Column I) ;

Column (V): predicted enthalpy of formation of anhydrous salt with parameters $\Delta_H O^\circ M_i^{Z_i+} (c)$;

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