

Data descriptor

Geochemical modelling and seasonal hydrogeochemical processes of the open-pit groundwater at O’Kiep, Namaqualand, South Africa

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Abstract: To assess dissolution, precipitation processes and saturation indices (SI) of some mineral phases, PHREEQC modelling software was used to assess these different geochemical processes and to elucidate reactive minerals of the open-pit groundwater (OPGW) in O’Kiep, Namaqualand, South Africa. Equilibrium constants were not fixed into the coding of the software PHREEQC, to accommodate equilibrium constant changes, and PHREEQC user input file manipulation. The SI of less than zero implied that the OPGW was undersaturated and that mineral dissolution was required to reach equilibrium. The data of the hydrogeochemical analysis indicated that the sources of ions into the OPGW are largely from the dissolution and leaching of mine waste and tailings including runoffs during the wet season, with the underlying fracturing of rocks, cation exchanges and other anthropogenic activities making a contribution. Additionally, climatic seasonality significantly influenced the OPGW hydrogeochemistry, indicating that the hydrological processes which control changes were dilution and mobilization of potentially toxic elements (PTEs). The data set generated showed that the OPGW chemistry was mainly influenced by evaporation, ion exchange, silicate weathering and dissolution of minerals including precipitation. Overall, this dataset details hydrogeochemical processes that are responsible for seasonal variations in the OPGW chemistry.

Keywords: Hydrogeochemical processes, Geochemical modelling, Open-pit groundwater, PHREEQC, O’Kiep

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Specification Table

Subject area	Hydrogeochemical modelling, Open-pit groundwater , PHREEQC
More specific subject area	Hydrogeochemical modelling
Type of data	Table
How data was acquired	PHREEQC Version 3 is a computer program for speciation, batch-reaction, one-Dimensional transport, and inverse geochemical computations and modelling, for reactions in water to understand water, sediments and aquifer rock interactions. Equilibrium constants are not fixed into the coding of the software to accommodate changes in the equilibrium constants. PHREEQC and EQ3/6 enables the user to manipulate the database and input files to change equilibrium constants when needed.
Data format	Raw Data
Experimental features	O'Kiep (open-pit groundwater), South Africa [29°35'55.4"S 17°52'48.2"E] Sample preparation: Cape Peninsula University of Technology, <i>BioERG</i> laboratory, Cape Town, South Africa [-33°93'0950"S, 18°43'3531"E]
Data source and location	Groundwater from an open-pit in O'Kiep, Namaqualand, South Africa [29°35'55.4"S 17°52'48.2"E]
Data accessibility	PHREEQC software was developed by the US Geological Survey with speciation and reaction path program features. The software makes use of a C++ programming language to compute speciation, solubility, reaction pathways and inverse geochemical mass balance modelling. The program does consider analytical uncertainties. PHREEQC has no licence obligations and permission is not required from the USGS. PHREEQC is downloadable from https://www.usgs.gov/core-science-systems/ngp/national-hydrography

Value of the data

- Several areas in Namaqualand are affected by elevated levels of PTEs) with their source being attributed to groundwater contamination; moreover, the processes contributing to changes in the quality of the open-pit groundwater in O'Kiep has not been modelled before.
- The hydrochemical characterization of variations in OPGW was an essential first step for effective management of groundwater resources in O'Kiep (Erdogan *et al.*, 2017)

with PHREEQC modelling being regarded as a vital tool to elucidate geochemical processes involved. PHREEQC software was successfully used to generate hydrogeochemical data of the OPGW to determine factors that control the groundwater chemistry and the hydrogeochemical evolution of the water, a first attempt for the OPGW in O’Kiep. Additionally, future research studies require the use of geochemical modelling to perform speciation, solubility, reaction path and inverse mass balance modelling. Estimation of chemical reactivity in the form of water-rock interactions is needed to understand hydrogeochemical changes in the semi-pocketed aquifer in the region are needed.

- This research data provides crucial simulation model information for chemically reactive transport processes to optimally characterize the OPGW in O’Kiep.

Data

This study presents the hydrogeochemical analysis of the granite and granitic gneiss open-pit groundwater (OPGW) in the arid O’Kiep. OPGW samples were collected in the dry (n=5) and wet (n=5) seasons downstream from a closed metalliferous mine. The seasonal variation of species observed was due to changes in the hydrogeochemical quality of the OPGW between the two seasons. The interaction between the OPGW and rock mineralogy controls the geochemistry of the OPGW. PHREEQC modelling software approach allowed for simulation and characterization of the primary physical and chemical processes influencing the OPGW’s quality. The mineral equilibrium calculation predicted the composition of the groundwater contaminated by various minerals predicting reactive mineral mechanisms. The variations observed between different seasons were attributed geological matrix interaction between major cations and anions.

References

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Table1: Statistical summary of saturation indices of minerals in groundwater using PHREEQC

Phase	SI	log IAP	log K(291 K)	log K(291 K, 1 atm)
(Co(NH ₃) ₅ Cl)(NO ₃) ₂	172.61	-166.35	6.26	(Co(NH ₃) ₅ Cl)(NO ₃) ₂
(Co(NH ₃) ₅ Cl)Cl ₂	-46.17	-41.62	4.55	(Co(NH ₃) ₅ Cl)Cl ₂
(Co(NH ₃) ₅ OH ₂)Cl ₃	-53.47	-41.64	11.83	(Co(NH ₃) ₅ OH ₂)Cl ₃
(Co(NH ₃) ₆)(NO ₃) ₃	246.96	-229.03	17.93	(Co(NH ₃) ₆)(NO ₃) ₃
(Co(NH ₃) ₆)Cl ₃	-62.1	-41.94	20.16	(Co(NH ₃) ₆)Cl ₃
(NH ₄) ₂ CrO ₄	-56.45	-56.08	0.37	(NH ₄) ₂ CrO ₄
(NH ₄) ₂ SeO ₄	-38.51	-38.06	0.45	(NH ₄) ₂ SeO ₄
(VO) ₃ (PO ₄) ₂	-35.27	-60.37	-25.1	(VO) ₃ (PO ₄) ₂
Al(OH) ₃ (am)	-6.61	4.62	11.23	Al(OH) ₃
Al ₂ O ₃	-11.37	9.28	20.65	Al ₂ O ₃
Al ₄ (OH) ₁₀ SO ₄	-12.76	9.94	22.7	Al ₄ (OH) ₁₀ SO ₄
AlAsO ₄ :2H ₂ O	-12.65	-7.85	4.8	AlAsO ₄ :2H ₂ O
AlOHSO ₄	-0.68	-3.91	-3.23	AlOHSO ₄
AlSb	109.2	-43.57	65.62	AlSb
Alunite	-2.56	-3.15	-0.59	KAl ₃ (SO ₄) ₂ (OH) ₆
Anhydrite	-0.21	-4.54	-4.33	CaSO ₄
Anilite	2.69	-29.89	-32.58	Cu _{0.25} Cu _{1.5} S
Antlerite	-7.28	1.51	8.79	Cu ₃ (OH) ₄ SO ₄
Aragonite	-4.19	-12.44	-8.25	CaCO ₃
Arsenolite	-24.15	-27.15	-2.99	As ₄ O ₆
Artinite	-18.14	-8.07	10.07	MgCO ₃ :Mg(OH) ₂ :3H ₂ O
As ₂ O ₅	-31.72	-24.92	6.79	As ₂ O ₅
Atacamite	-6.26	1.5	7.75	Cu ₂ (OH) ₃ Cl
Azurite	-6.28	-22.82	-16.54	Cu ₃ (OH) ₂ (CO ₃) ₂
Bianchite	-7.83	-9.59	-1.76	ZnSO ₄ :6H ₂ O
Birnessite	-27.63	-9.54	18.09	MnO ₂
Bixbyite	-32.63	-32.79	-0.16	Mn ₂ O ₃
Blaubleil	-2.47	-26.63	-24.16	Cu _{0.9} Cu _{0.2} S
Blaubleill	-0.85	-28.13	-27.28	Cu _{0.6} Cu _{0.8} S
Boehmite	-4.4	4.63	9.03	AlOOH
Breithauptite	-20.4	-39.29	-18.89	NiSb
Brochantite	-11.15	4.86	16.01	Cu ₄ (OH) ₆ SO ₄
Brucite	-13.08	4.2	17.29	Mg(OH) ₂
Bunsenite	-10.77	2.07	12.83	NiO
Ca(VO ₃) ₂	-26.85	-20.86	5.99	Ca(VO ₃) ₂
Ca ₂ V ₂ O ₇	-34.97	-16.86	18.12	Ca ₂ V ₂ O ₇
Ca ₂ V ₂ O ₇ :2H ₂ O	-38.44	-16.89	21.55	Ca ₂ V ₂ O ₇ :2H ₂ O
Ca ₃ (AsO ₄) ₂ :4H ₂ O	-35.27	-12.97	22.3	Ca ₃ (AsO ₄) ₂ :4H ₂ O
Ca ₃ (PO ₄) ₂ (beta)	-13.5	-42.63	-29.13	Ca ₃ (PO ₄) ₂
Ca ₃ (VO ₄) ₂	-52.95	-12.85	40.1	Ca ₃ (VO ₄) ₂
Ca ₃ (VO ₄) ₂ :4H ₂ O	-52.78	-12.92	39.86	Ca ₃ (VO ₄) ₂ :4H ₂ O
Ca ₃ Sb ₂	230.23	-84.41	145.81	Ca ₃ Sb ₂
Ca ₄ H(PO ₄) ₃ :3H ₂ O	-18.92	-66	-47.08	Ca ₄ H(PO ₄) ₃ :3H ₂ O
CaCrO ₄	-49.26	-51.42	-2.16	CaCrO ₄

CaHPO ₄	-3.93	-23.32	-19.4	CaHPO ₄
CaHPO ₄ ·2H ₂ O	-4.27	-23.36	-19.08	CaHPO ₄ ·2H ₂ O
Calcite	-3.99	-12.44	-8.45	CaCO ₃
Calomel	-1.57	-19.83	-18.27	Hg ₂ Cl ₂
CaSeO ₃ ·2H ₂ O	-12.95	-10.06	2.89	CaSeO ₃ ·2H ₂ O
CaSeO ₄ ·2H ₂ O	-30.45	-33.44	-2.99	CaSeO ₄ ·2H ₂ O
Cd(OH) ₂	-14.91	-0.9	14.01	Cd(OH) ₂
Cd(OH) ₂ (am)	-14.96	-0.9	14.07	Cd(OH) ₂
Cd ₃ (OH) ₂ (SO ₄) ₂	-26.47	-19.76	6.71	Cd ₃ (OH) ₂ (SO ₄) ₂
Cd ₃ (OH) ₄ SO ₄	-33.78	-11.22	22.56	Cd ₃ (OH) ₄ SO ₄
Cd ₃ (PO ₄) ₂	-24.69	-57.29	-32.6	Cd ₃ (PO ₄) ₂
Cd ₄ (OH) ₆ SO ₄	-40.52	-12.12	28.4	Cd ₄ (OH) ₆ SO ₄
CdCl ₂	-10.71	-11.29	-0.59	CdCl ₂
CdCl ₂ ·1H ₂ O	-9.64	-11.31	-1.66	CdCl ₂ ·1H ₂ O
CdCl ₂ ·2.5H ₂ O	-9.39	-11.33	-1.94	CdCl ₂ ·2.5H ₂ O
CdF ₂	-18.36	-19.39	-1.03	CdF ₂
Cdmetal(alpha)	-28.4	-14.59	13.81	Cd
Cdmetal(gamma)	-28.5	-14.59	13.91	Cd
CdOHCl	-9.75	-6.1	3.66	CdOHCl
CdSb	-41.81	-42.24	-0.44	CdSb
CdSe	9.32	-11.18	-20.49	CdSe
CdSeO ₄ ·2H ₂ O	-36.47	-38.32	-1.85	CdSeO ₄ ·2H ₂ O
CdSO ₄	-9.46	-9.43	0.03	CdSO ₄
CdSO ₄ ·1H ₂ O	-7.84	-9.45	-1.6	CdSO ₄ ·1H ₂ O
Cd ₅ O ₄ ·2.67H ₂ O	-7.67	-9.47	-1.8	CdSO ₄ ·2.67H ₂ O
CH ₄ (g)	-29.27	-71.31	-42.04	CH ₄
Chalcanthite	-2.6	-5.27	-2.66	CuSO ₄ ·5H ₂ O
Chalcocite	4.43	-31.14	-35.57	Cu ₂ S
Chalcopyrite	-17.24	-53.09	-35.85	CuFeS ₂
Cinnabar	-2.38	-49.06	-46.68	HgS
Claudetite	-23.86	-27.15	-3.28	As ₄ O ₆
Co(OH) ₂	-11.97	1.12	13.09	Co(OH) ₂
Co(OH) ₃	-22.48	-24.43	-1.95	Co(OH) ₃
CO ₂ (g)	1.72	-16.45	-18.16	CO ₂
Co ₃ (AsO ₄) ₂	-34.55	-21.51	13.03	Co ₃ (AsO ₄) ₂
Co ₃ (PO ₄) ₂	-16.54	-51.23	-34.69	Co ₃ (PO ₄) ₂
Co ₃ O ₄	-37.6	-47.68	-10.08	Co ₃ O ₄
CoCl ₂	-17.85	-9.27	8.58	CoCl ₂
CoCl ₂ ·6H ₂ O	-11.88	-9.37	2.51	CoCl ₂ ·6H ₂ O
CoCO ₃	-5.38	-15.31	-9.93	CoCO ₃
CoF ₂	-16	-17.37	-1.37	CoF ₂
CoF ₃	-51.2	-52.18	-0.98	CoF ₃
CoFe ₂ O ₄	-3.58	-6.49	-2.91	CoFe ₂ O ₄
CoHPO ₄	-7.13	-26.19	-19.06	CoHPO ₄
CoO	-12.86	1.14	14	CoO
CoS(alpha)	-20.91	-28.35	-7.44	CoS

CoS(beta)	-17.28	-28.35	-11.07	CoS
CoSe	7.04	-9.16	-16.2	CoSe
CoSeO ₃	-14.21	-12.89	1.32	CoSeO ₃
CoSeO ₄ :6H ₂ O	-34.84	-36.37	-1.53	CoSeO ₄ :6H ₂ O
CoSO ₄	-10.52	-7.41	3.11	CoSO ₄
CoSO ₄ :6H ₂ O	-5.03	-7.51	-2.48	CoSO ₄ :6H ₂ O
Covellite	-3.45	-26.13	-22.68	CuS
Cr(OH) ₂	-23.12	-12.16	10.96	Cr(OH) ₂
Cr(OH) ₃	-9.69	-8.24	1.45	Cr(OH) ₃
Cr(OH) ₃ (am)	-7.49	-8.24	-0.75	Cr(OH) ₃
Cr ₂ O ₃	-14.26	-16.43	-2.16	Cr ₂ O ₃
CrCl ₂	-37.08	-22.56	14.52	CrCl ₂
CrCl ₃	-39.41	-23.83	15.58	CrCl ₃
CrF ₃	-24.73	-35.98	-11.25	CrF ₃
Crmetal	-57	-25.85	31.15	Cr
CrO ₃	-52.23	-55.42	-3.19	CrO ₃
Cryolite	-12.46	-46.45	-33.99	Na ₃ AlF ₆
Cu(OH) ₂	-5.55	3.35	8.89	Cu(OH) ₂
Cu(SbO ₃) ₂	-28.61	16.6	45.21	Cu(SbO ₃) ₂
Cu ₂ (OH) ₃ NO ₃	-70.4	-60.87	9.53	Cu ₂ (OH) ₃ NO ₃
Cu ₂ Sb:3H ₂ O	-9.94	-45.73	-35.79	Cu ₂ Sb:3H ₂ O
Cu ₂ Se(alpha)	34.68	-11.95	-46.63	Cu ₂ Se
Cu ₂ SO ₄	-8.33	-10.2	-1.88	Cu ₂ SO ₄
Cu ₃ (AsO ₄) ₂ :2H ₂ O	-20.97	-14.87	6.1	Cu ₃ (AsO ₄) ₂ :2H ₂ O
Cu ₃ (PO ₄) ₂	-7.7	-44.55	-36.85	Cu ₃ (PO ₄) ₂
Cu ₃ (PO ₄) ₂ :3H ₂ O	-9.48	-44.6	-35.12	Cu ₃ (PO ₄) ₂ :3H ₂ O
Cu ₃ Sb	-6.91	-50.7	-43.79	Cu ₃ Sb
Cu ₃ Se ₂	45.92	-18.89	-64.81	Cu ₃ Se ₂
CuCO ₃	-1.58	-13.08	-11.5	CuCO ₃
CuCrO ₄	-46.62	-52.06	-5.44	CuCrO ₄
CuF	-5.11	-10.08	-4.97	CuF
CuF ₂	-16.52	-15.15	1.37	CuF ₂
CuF ₂ :2H ₂ O	-10.69	-15.18	-4.49	CuF ₂ :2H ₂ O
Cumetal	1.35	-7.68	-9.03	Cu
CuOCuSO ₄	-12.66	-1.82	10.84	CuOCuSO ₄
Cupricferrite	-11.07	-4.27	6.8	CuFe ₂ O ₄
Cuprite	-0.73	-1.66	-0.93	Cu ₂ O
Cuprousferrite	4.21	-4.64	-8.86	CuFeO ₂
CuSe	26.64	-6.93	-33.57	CuSe
CuSe ₂	30.39	-3.52	-33.91	CuSe ₂
CuSeO ₃ :2H ₂ O	-11.35	-10.7	0.65	CuSeO ₃ :2H ₂ O
CuSeO ₄ :5H ₂ O	-31.69	-34.13	-2.44	CuSeO ₄ :5H ₂ O
CuSO ₄	-8.41	-5.18	3.22	CuSO ₄
Diaspore	-2.64	4.63	7.27	AlOOH
Djurleite	3.88	-30.81	-34.7	Cu _{0.066} Cu _{1.868} S
Dolomite(disorde	-8	-24	.67 -16	.36 CaMg(CO ₃) ₂

Dolomite(ordered	-7.73	-24.67	-16.94	CaMg(CO ₃) ₂
Epsomite	-2.27	-4.44	-2.17	MgSO ₄ ·7H ₂ O
FCO ₃ Apatite	-20.34	-135.38	115.04	Ca ₉ .316Na _{0.36} Mg _{0.144} (PO ₄) ₄ .8(CO ₃)1.2F2.48
Fe(OH) ₂	-11.05	2.51	13.56	Fe(OH) ₂
Fe(OH)2.7Cl.3	-2.36	-5.4	-3.04	Fe(OH) ₂ .7Cl.3
Fe(VO ₃) ₂	-18.86	-22.34	-3.48	Fe(VO ₃) ₂
Fe ₂ (OH) ₄ SeO ₃	-23.25	-21.69	1.55	Fe ₂ (OH) ₄ SeO ₃
Fe ₂ (SeO ₃) ₃ :2H ₂ O	-29.13	-49.76	-20.63	Fe ₂ (SeO ₃) ₃ :2H ₂ O
Fe ₂ (SO ₄) ₃	-30.48	-33.27	-2.8	Fe ₂ (SO ₄) ₃
Fe ₃ (OH) ₈	-25.39	-5.17	20.22	Fe ₃ (OH) ₈
FeAsO ₄ :2H ₂ O	-16.71	-16.31	0.4	FeAsO ₄ :2H ₂ O
FeCr ₂ O ₄	-21.64	-13.9	7.74	FeCr ₂ O ₄
Ferrihydrite	-7.32	-3.84	3.48	Fe(OH) ₃
Ferroselite	14.42	-4.36	-18.78	FeSe ₂
FeS(ppt)	-24.05	-26.96	-2.91	FeS
FeSe	3.24	-7.77	-11.01	FeSe
Fluorite	-3.97	-14.51	-10.53	CaF ₂
Gibbsite	-4.04	4.62	8.66	Al(OH) ₃
Goethite	-4.55	-3.82	0.73	FeOOH
Goslarite	-7.54	-9.61	-2.07	ZnSO ₄ :7H ₂ O
Greenockite	-15.8	-30.37	-14.57	CdS
Greigite	-78.02	-123.06	-45.03	Fe ₃ S ₄
Gypsum	0.04	-4.57	-4.61	CaSO ₄ :2H ₂ O
H-Jarosite	-17.41	-28.61	-11.21	(H ₃ O)Fe ₃ (SO ₄) ₂ (OH) ₆
H ₂ S(g)	-21.49	-29.5	-8.01	H ₂ S
H ₂ Se(g)	-5.41	-10.31	-4.9	H ₂ Se
Halite	-5.31	-3.72	1.59	NaCl
Hausmannite	-41.4	21.26	62.66	Mn ₃ O ⁴
Hematite	-6.71	-7.63	-0.92	Fe ₂ O ₃
Hercynite	-12.3	11.81	24.11	FeAl ₂ O ₄
Hg(CH ₃) ₂ (g)	-86.61	-162.18	-75.57	Hg(CH ₃) ₂
Hg(g)	-3.61	-11.56	-7.96	Hg
Hg(OH) ₂	-16.09	-19.59	-3.5	Hg(OH) ₂
Hg ₂ (g)	-7.95	-23.13	-15.18	Hg ₂ (g)
Hg ₂ (OH) ₂	-14.7	-9.44	5.26	Hg ₂ (OH) ₂
Hg ₂ CO ₃	-9.64	-25.87	-16.22	Hg ₂ CO ₃
Hg ₂ CrO ₄	-56.15	-64.85	-8.7	Hg ₂ CrO ₄
Hg ₂ F ₂	-17.64	-27.93	-10.29	Hg ₂ F ₂
Hg ₂ HPO ₄	-11.98	-36.75	-24.77	Hg ₂ HPO ₄
Hg ₂ S	-26.96	-38.91	-11.95	Hg ₂ S
Hg ₂ SeO ₃	-18.8	-23.45	-4.66	Hg ₂ SeO ₃
Hg ₂ SO ₄	-11.82	-17.97	-6.15	Hg ₂ SO ₄
Hg ₃ O ₂ CO ₃	-45.48	-75.16	-29.68	Hg ₃ O ₂ CO ₃
HgCl(g)	-30.04	-9.92	20.12	HgCl
HgCl ₂	-8.3	-29.98	-21.68	HgCl ₂
HgF(g)	-47.63	-13.97	33.66	HgF

HgF ₂ (g)	-51.29	-38.08	13.21	HgF ₂
Hgmetal(l)	2.21	-11.56	-13.77	Hg
HgSe	25.83	-29.87	-55.69	HgSe
HgSeO ₃	-21.17	-33.6	-12.43	HgSeO ₃
HgSO ₄	-18.64	-28.12	-9.48	HgSO ₄
Huntite	-19.57	-49.12	-29.55	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-36.85	-44.77	-7.92	Mg ₅ (CO ₃) ₄ (OH) ₂ :4H ₂ O
Hydroxylapatite	-17.61	-61.94	-44.33	Ca ₅ (PO ₄) ₃ OH
K-Alum	-7.29	-12.58	-5.29	KAl(SO ₄) ₂ :12H ₂ O
K-Jarosite	-14.23	-28.52	-14.29	KFe ₃ (SO ₄) ₂ (OH) ₆
K ₂ Cr ₂ O ₇	-93.15	-110.71	-17.56	K ₂ Cr ₂ O ₇
K ₂ CrO ₄	-54.7	-55.28	-0.58	K ₂ CrO ₄
K ₂ SeO ₄	-36.54	-37.27	-0.73	K ₂ SeO ₄
Langite	-13.29	4.84	18.13	Cu ₄ (OH) ₆ SO ₄ :H ₂ O
Lepidocrocite	-5.19	-3.82	1.37	FeOOH
Lime	-29.44	4.01	33.45	CaO
Mackinawite	-23.36	-26.96	-3.6	FeS
Maghemite	-14.02	-7.63	6.39	Fe ₂ O ₃
Magnesioferrite	-21.35	-3.41	17.94	Fe ₂ MgO ₄
Magnesite	-4.69	-12.23	-7.54	MgCO ₃
Magnetite	-9.31	-5.1	4.21	Fe ₃ O ₄
Malachite	-4.13	-9.74	-5.6	Cu ₂ (OH) ₂ CO ₃
Manganite	-15.98	9.36	25.34	MnOOH
Melanothallite	-13.55	-7.05	6.5	CuCl ₂
Melanterite	-3.85	-6.13	-2.29	FeSO ₄ :7H ₂ O
Metacinnabar	-2.98	-49.06	-46.08	HgS
Mg(OH) ₂ (active)	-14.59	4.2	18.79	Mg(OH) ₂
Mg(VO ₃) ₂	-32.46	-20.65	11.81	Mg(VO ₃) ₂
Mg ₂ Sb ₃	176.62	-101.94	74.68	Mg ₂ Sb ₃
Mg ₂ V ₂ O ₇	-43.78	-16.43	27.35	Mg ₂ V ₂ O ₇
Mg ₃ (PO ₄) ₂	-18.71	-41.99	-23.28	Mg ₃ (PO ₄) ₂
MgCr ₂ O ₄	-29.1	-12.21	16.9	MgCr ₂ O ₄
MgCrO ₄	-56.93	-51.21	5.72	MgCrO ₄
MgF ₂	-6.19	-14.29	-8.1	MgF ₂
MgHPO ₄ :3H ₂ O	-4.99	-23.16	-18.18	MgHPO ₄ :3H ₂ O
MgSeO ₃ :6H ₂ O	-12.95	-9.91	3.04	MgSeO ₃ :6H ₂ O
MgSeO ₄ :6H ₂ O	-32.09	-33.29	-1.2	MgSeO ₄ :6H ₂ O
Mirabilite	-4.33	-5.75	-1.42	Na ₂ SO ₄ :10H ₂ O
Mn(VO ₃) ₂	-27.61	-22.35	5.26	Mn(VO ₃) ₂
Mn ₂ (SO ₄) ₃	-53.35	-58.43	-5.08	Mn ₂ (SO ₄) ₃
Mn ₂ Sb	111.11	-50.03	61.08	Mn ₂ Sb
Mn ₃ (AsO ₄) ₂ :8H ₂ O	-30	-17.5	12.5	Mn ₃ (AsO ₄) ₂ :8H ₂ O
Mn ₃ (PO ₄) ₂	-23.23	-47.09	-23.86	Mn ₃ (PO ₄) ₂
MnCl ₂ :4H ₂ O	-10.71	-7.96	2.76	MnCl ₂ :4H ₂ O
MnHPO ₄	0.59	-24.81	-25.4	MnHPO ₄
MnS(grn)	-27.26	-26.97	0.29	MnS

MnS(pnk)	-30.31	-26.97	3.34	MnS
MnSb	-61.62	-64.61	-2.99	MnSb
MnSe	-11.66	-7.78	3.88	MnSe
MnSeO ₃	-12.64	-11.51	1.13	MnSeO ₃
MnSeO ₃ :2H ₂ O	-12.49	-11.54	0.95	MnSeO ₃ :2H ₂ O
MnSeO ₄ :5H ₂ O	-32.92	-34.97	-2.05	MnSeO ₄ :5H ₂ O
MnSO ₄	-8.86	-6.03	2.83	MnSO ₄
Monteponite	-16.39	-0.88	15.5	CdO
Montroydite	-16.08	-19.57	-3.49	HgO
Morenosite	-4.4	-6.6	-2.19	NiSO ₄ :7H ₂ O
Na-Jarosite	-16.5	-27.11	-10.61	NaFe ₃ (SO ₄) ₂ (OH) ₆
Na ₂ Cr ₂ O ₇	-97.91	-107.89	-9.98	Na ₂ Cr ₂ O ₇
Na ₂ CrO ₄	-55.47	-52.46	3.01	Na ₂ CrO ₄
Na ₂ SeO ₃ :5H ₂ O	-21.45	-11.15	10.3	Na ₂ SeO ₃ :5H ₂ O
Na ₂ SeO ₄	-35.73	-34.45	1.28	Na ₂ SeO ₄
Na ₃ Sb	139.9	-43.77	96.13	Na ₃ Sb
Na ₃ VO ₄	-45.39	-7.99	37.4	Na ₃ VO ₄
Na ₄ V ₂ O ₇	-57.12	-18.94	38.18	Na ₄ V ₂ O ₇
Nantokite	0.86	-6.03	-6.9	CuCl
NaSb	-56.55	-33.03	23.53	NaSb
Natron	-12.08	-13.65	-1.57	Na ₂ CO ₃ :10H ₂ O
NaVO ₃	-14.93	-10.95	3.98	NaVO ₃
Nesquehonite	-7.7	-12.28	-4.58	MgCO ₃ :3H ₂ O
Ni(OH) ₂	-11.12	2.05	13.17	Ni(OH) ₂
Ni ₃ (AsO ₄) ₂ :8H ₂ O	-34.56	-18.86	15.7	Ni ₃ (AsO ₄) ₂ :8H ₂ O
Ni ₃ (PO ₄) ₂	-17.14	-48.44	-31.3	Ni ₃ (PO ₄) ₂
Ni ₄ (OH) ₆ SO ₄	-32.33	-0.33	32	Ni ₄ (OH) ₆ SO ₄
NiCO ₃	-7.67	-14.38	-6.71	NiCO ₃
NiS(alpha)	-21.82	-27.42	-5.6	NiS
NiS(beta)	-16.32	-27.42	-11.1	NiS
NiS(gamma)	-14.62	-27.42	-12.8	NiS
NiSe	9.47	-8.23	-17.7	NiSe
NiSeO ₃ :2H ₂ O	-14.93	-12	2.93	NiSeO ₃ :2H ₂ O
NiSeO ₄ :6H ₂ O	-33.92	-35.44	-1.52	NiSeO ₄ :6H ₂ O
Nsutite	-27.04	-9.54	17.5	MnO ₂
O ₂ (g)	-57.89	27.42	85.3	O ₂
Orpiment	-39.61	-102.04	-62.42	As ₂ S ₃
Otavite	-5.33	-17.33	-12	CdCO ₃
Periclase	-17.95	4.22	22.17	MgO
Portlandite	-19.31	3.99	23.3	Ca(OH) ₂
Pyrite	-24.04	-42.74	-18.7	FeS ₂
Pyrochroite	-13.07	2.5	15.57	Mn(OH) ₂
Pyrolusite	-26.21	16.23	42.43	MnO ₂
Realgar	-22.89	-43.13	-20.24	AsS
Retgersite	-4.52	-6.58	-2.06	NiSO ₄ :6H ₂ O
Rhodochrosite	-3.36	-13.93	-10.57	MnCO ₃

Sb(OH) ₃	0.11	-7.11	-7.23	Sb(OH) ₃
Sb ₂ O ₄	-4.14	-0.47	3.67	Sb ₂ O ₄
Sb ₂ O ₅	-25.71	-35.38	-9.67	Sb ₂ O ₅
Sb ₂ Se ₃	24.02	-45.07	-69.09	Sb ₂ Se ₃
Sb ₄ O ₆ (cubic)	-9.86	-28.36	-18.5	Sb ₄ O ₆
Sb ₄ O ₆ (orth)	-10.31	-28.36	-18.05	Sb ₄ O ₆
SbCl ₃	-23.41	-22.71	0.71	SbCl ₃
SbF ₃	-24.66	-34.86	-10.2	SbF ₃
Sbmetal	-15.64	-27.65	-12.01	Sb
SbO ₂	3.28	-24.54	-27.82	SbO ₂
Semetal(am)	10.56	3.41	-7.15	Se
Semetal(hex)	11.18	3.41	-7.77	Se
Senarmontite	-1.69	-14.18	-12.48	Sb ₂ O ₃
SeO ₂	-14.15	-14.03	0.12	SeO ₂
SeO ₃	-59.02	-37.41	21.61	SeO ₃
Siderite	-3.74	-13.92	-10.18	FeCO ₃
Smithsonite	-7.45	-17.39	-9.94	ZnCO ₃
Sphalerite	-18.87	-30.44	-11.57	ZnS
Spinel	-24.85	13.5	38.35	MgAl ₂ O ₄
Stibnite	-51.05	-102.64	-51.6	Sb ₂ S ₃
Strengite	-4.81	-31.17	-26.36	FePO ₄ ·2H ₂ O
Sulfur	-13.7	-15.78	-2.08	S
Tenorite	-4.53	3.36	7.9	CuO
Thenardite	-5.94	-5.59	0.36	Na ₂ SO ₄
Thermonatrite	-14.18	-13.5	0.68	Na ₂ CO ₃ ·H ₂ O
V(OH) ₃	-10.68	-3.09	7.59	V(OH) ₃
V ₂ O ₅	-23.38	-24.87	-1.49	V ₂ O ₅
V ₃ O ₅	-21.66	-19.44	2.22	V ₃ O ₅
V ₄ O ₇	-29.17	-21.35	7.82	V ₄ O ₇
V ₆ O ₁₃	-40.11	-102.02	-61.91	V ₆ O ₁₃
Valentinite	-5.62	-14.18	-8.55	Sb ₂ O ₃
VCl ₂	-39.75	-20.33	19.42	VCl ₂
VCl ₃	-42.81	-18.68	24.13	VCl ₃
VF ₄	-54.63	-38.93	15.7	VF ₄
Vivianite	-11.19	-47.19	-36	Fe ₃ (PO ₄) ₂ ·8H ₂ O
Vmetal	-68.66	-23.63	45.03	V
VO	-25.12	-9.92	15.19	VO
VO(OH) ₂	-7.08	-1.93	5.15	VO(OH) ₂
VO ₂ Cl	-20.64	-17.64	3	VO ₂ Cl
VOCl	-19.83	-8.27	11.56	VOCl
VOCl ₂	-25.54	-12.32	13.22	VOCl ₂
VOSO ₄	-14.4	-10.46	3.95	VOSO ₄
Wurtzite	-21.4	-30.44	-9.03	ZnS
Zincite	-12.63	-0.95	11.68	ZnO
Zincosite	-13.74	-9.49	4.25	ZnSO ₄
Zn(NO ₃) ₂ ·6H ₂ O	139.4	-136.18	3.22	Zn(NO ₃) ₂ ·6H ₂ O

Zn(OH) ₂	-13.16	-0.96	12.2	Zn(OH) ₂
Zn(OH) ₂ (am)	-13.75	-0.96	12.79	Zn(OH) ₂
Zn(OH) ₂ (beta)	-13.04	-0.96	12.08	Zn(OH) ₂
Zn(OH) ₂ (epsilon)	-12.81	-0.96	11.85	Zn(OH) ₂
Zn(OH) ₂ (gamma)	-12.7	-0.96	11.73	Zn(OH) ₂
Zn ₂ (OH) ₂ SO ₄	-17.96	-10.46	7.5	Zn ₂ (OH) ₂ SO ₄
Zn ₂ (OH) ₃ Cl	-22.31	-7.12	15.19	Zn ₂ (OH) ₃ Cl
Zn ₃ (AsO ₄) ₂ ·2.5H ₂ O	-41.46	-27.81	13.65	Zn ₃ (AsO ₄) ₂ ·2.5H ₂ O
Zn ₃ (PO ₄) ₂ ·4H ₂ O	-22.13	-57.55	-35.42	Zn ₃ (PO ₄) ₂ ·4H ₂ O
Zn ₃ O(SO ₄) ₂	-39.85	-19.94	19.91	Zn ₃ O(SO ₄) ₂
Zn ₄ (OH) ₆ SO ₄	-40.78	-12.38	28.4	Zn ₄ (OH) ₆ SO ₄
Zn ₅ (OH) ₈ Cl ₂	-53.71	-15.21	38.5	Zn ₅ (OH) ₈ Cl ₂
ZnCl ₂	-18.69	-11.36	7.33	ZnCl ₂
ZnCO ₃ ·1H ₂ O	-7.15	-17.41	-10.26	ZnCO ₃ ·1H ₂ O
ZnF ₂	-19.15	-19.46	-0.3	ZnF ₂
Znmetal	-41.04	-14.66	26.38	Zn
ZnO(active)	-12.48	-0.95	11.53	ZnO
ZnS(am)	-21.32	-30.44	-9.11	ZnS
ZnSb	-53.53	-42.31	11.23	ZnSb
ZnSe	3.26	-11.24	-14.5	ZnSe
ZnSeO ₄ ·6H ₂ O	-36.93	-38.45	-1.52	ZnSeO ₄ ·6H ₂ O
ZnSO ₄ ·1H ₂ O	-9.04	-9.51	-0.47	ZnSO ₄ ·1H ₂ O