**data descriptor**

Geochemical modelling of groundwater in the Namaqualand region, South Africa

Innocentia G. Erdogan123\*, Alseno Mosai4, Seteno K.O. Ntwampe1, Elvis Fosso-Kankeu1, Frans B. Waanders1

**Abstract:**

Namaqualand is one of the aridest areas in South Africa. In recent years, rapid development has created a higher demand for water which is increasingly fulfilled by groundwater abstraction. Comprehensive information of geochemical evolution of groundwater quality can improve the understanding of hydrochemical characteristics, and promote sustainable development and effective management of groundwater resources. The study aims were to use PHREEQC model to determine hydrogeochemical characteristics of groundwater, to determine how groundwater has deteriorated of time and to identify the major phases that control groundwater in such arid region. The model output showed phases that are governing the groundwater chemistry in this area. The geochemical reactions responsible for the evolution of groundwater chemistry along the flow path were the dissolution of the carbonate minerals such as aragonite, Ca3(PO4)2, calcite dolomite, ferrihydrite and vaterite keep gradually from undersaturation to supersaturating status and vice versa happed for Cd(CO3), Cr(OH)3. The precipitation of anapaite, chloroapatite, chromite, Cr2O3Fe5(OH)(PO4)3, ferryhydrite, goethite, hematite, hydroxyapatite, lepidocrocite, maghemite, magnetite. In contrast, magnesite changed from undersaturated to equilibrium phase. The SI of gypsum, siderite and halite remained undersaturated, indicating that these minerals may be subject to continuous dissolution. Groundwater hydrogeochemical evolution is mainly controlled by carbonate mineral dissolutions, cation exchange, precipitation and weathering.

**Keywords:** Hydrogeochemical processes, geochemical modelling, groundwater quality, PHREEQC, Namaqualand.

1I.G. Erdogan, E. Fosso-Kankeu, Seteno K.O. Ntwampe, and F. Waanders are with the Water Pollution Monitoring and Remediation Initiatives Research Group (WPMRIRG) in the CoE of C-based fuels School of Chemical and Minerals Engineering, North-West University, Potchefstroom, South Africa.

2I.G. Erdogan is with the Bioresource Engineering Research Group (BioERG), Cape Peninsula University of Technology, Cape Town, South Africa

3 I.G. Erdogan are with the Faculty of Engineering and the Built Environment, Chemical Engineering Department, Cape Peninsula University of Technology, Cape Town, South Africa.

4 Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa*.*

\*Corresponding author. +27 (18) 299 1659; Email: Elvis.FossoKankeu@nwu.ac.za

## **specification table**

|  |  |
| --- | --- |
| Subject area | Hydrogeochemical modelling, geohydrology, groundwater quality, 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 modelling for reactions in water to understand groundwater and aquifer rock interactions. Equilibrium constants were not fixed into the coding of the software to accommodate variations of the equilibrium constants. PHREEQC and EQ3/6 enable the user to manipulate the database and input files to change equilibrium constants when desired. |
| Data format | Raw Data |
| Experimental features | Namaqualand, South Africa [30°5'16.0692''S 17°34' 50.4768''E]Sample preparation: Cape Peninsula University of Technology, *BioERG* laboratory, Cape Town, South Africa[-33°93′0950″S, 18°43′3531″E] |
| Data source and location | Groundwater from boreholes in Namaqualand, South Africa[30°5'16.0692''S 17°34' 50.4768''E] |
| Data accessibility | The US Geological Survey developed PHREEQC software 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 potentially toxic elements (PTE's) with their source being attributed to groundwater contamination.
* In the study of Leshomo (2011), it was reported that the hydrochemistry of groundwater indicates that there is an evolution taking place. The processes contributing to changes in the borehole water quality in Namaqualand have not been modelled in the past.
* The hydrochemical characterisation of borehole water was an essential stage for effective management of groundwater resources in Namaqualand by Erdogan *et al.* (2019) and Abiye and Leshomo (2013); with PHREEQC modelling being regarded as a vital tool to elucidate the geochemical processes involved.
* PHREEQC results are of great significance for understanding the regional hydrochemical evolution of groundwater.
* The research data will assist in determining rock-water interactions and the hydrochemical evolution of groundwater and resolve hydrogeological challenges in this area.
* The data will provide critical knowledge on groundwater evolution with the change in environmental and societal conditions.

## **data**

This study presents the hydrogeochemical analysis of the groundwater in the arid Namaqualand. Groundwater samples were collected from eight boreholes by Erdogan *et al.* (2019) while the other data were extracted from the study published by Abiye and Leshomo (2013) as shown in Table 1 and most of the boreholes in the area are from fractured basement aquifers. PHREEQC was used to perform an aqueous geochemical calculation that has capabilities for saturation index (SI) and speciation calculations in a batch-reaction system (Parkhurst and Appelo, 2013, Parkhurst and Appelo, 1999). The interaction between the groundwater and rock mineralogy controls the geochemistry of the groundwater. PHREEQC modelling software approach allowed for simulation and characterisation of the hydrogeochemical processes influencing the groundwater quality. The composition of the groundwater contaminated by various minerals predicting reactive mineral mechanisms. The variations observed between different dataset were attributed to geological matrix interaction between significant anions and cations. The calculated SIs of particular phases are presented in Table 2.

Table 1: Represents the major ions from Namaqualand.

|  |  |  |
| --- | --- | --- |
| **Parameter** | **(Abiye and Leshomo, 2013)** | **(Erdogan *et al.*, 2019)** |
| pH | 7.11 | 8.1 |
| Eh  | 29.2 | -57.0 |
| T  | 22.1 | 15.0 |
| EC  | 2.04 | 241 |
| TDS  | 911 | 1793 |
| Alkalinity(Total)  | 179 | 134 |
| Na  | 224 | 243 |
| Mg  | 51.5 | 67.3 |
| K  | 5.69 | 15.3 |
| Ca  | 78.5 | 184 |
| Cl  | 447 | 470 |
| NO3  | 27.3 | 2.16 |
| PO4  | 1.41 | 0.50 |
| SO4  | 121 | 455 |
| Zn  | 0.81 | 0.00 |
| Fe  | 0.32 | 0.07 |
| Cd  | 9.77 | 0.003 |
| Cr  | 0.16 | 0.01 |

The units are all in mg/L with the exception of EC (mS/cm), Eh (mV), Temperature °C and pH

Table 2: Saturation index of minerals in groundwater

|  |  |
| --- | --- |
| **2013** | **2019**  |
| **Phase**  | **SI** | **log IAP** | **log K(295 K,1tm)** |  | **Phase** | **SI** |  **log IAP** | **log K(288 K, 1 atm)** |  |
| Anapaite | 1.64 | 6.66 | 5.02 | Ca2Fe(PO4)2:4H2O | Anapaite | 2.6 | 7.62 | 5.02 | Ca2Fe(PO4)2:4H2O |
| Anhydrite | -1.83 | -6.24 | -4.41 | Ca(SO4) | Anhydrite | -1.1 | -5.43 | -4.33 | Ca(SO4) |
| Antarcticite | -10.84 | -6.93 | 3.92 | CaCl2:6H2O | Antarcticite | -10.46 | -6.61 | 3.85 | CaCl2:6H2O |
| Aragonite | -0.49 | -8.78 | -8.29 | CaCO3 | Aragonite | 0.53 | -7.71 | -8.25 | CaCO3 |
| Arcanite | -9.15 | -11.04 | -1.89 | K2SO4 | Arcanite | -7.68 | -9.68 | -2.00 | K2SO4 |
| Artinite | -7.5 | 2.51 | 10.01 | Mg2(CO3)(OH)2:3H2O | Artinite | -5.17 | 5.36 | 10.53 | Mg2(CO3)(OH)2:3H2O |
| Bassanite | -2.35 | -6.24 | -3.89 | CaSO4:0.5H2O | Bassanite | -1.62 | -5.43 | -3.81 | CaSO4:0.5H2O |
| Bischofite | -11.37 | -6.89 | 4.47 | MgCl2:6H2O | Bischofite | -11.33 | -6.81 | 4.51 | MgCl2:6H2O |
| Bloedite | -11.24 | -13.59 | -2.35 | Na2Mg(SO4)2:4H2O | Bloedite | -10.11 | -12.46 | -2.35 | Na2Mg(SO4)2:4H2O |
| Brucite | -6.04 | 11.26 | 17.3 | Mg(OH)2 | Brucite | -4.51 | 13.28 | 17.79 | Mg(OH)2 |
| Brushite | -1.54 | -0.93 | 0.61 | Ca(HPO4):2H2O | Brushite | -1.53 | -0.88 | 0.64 | Ca(HPO4):2H2O |
| Burkeite | -23.94 | -24.71 | -0.77 | Na6(CO3)(SO4)2 | Burkeite | -21.97 | -22.74 | -0.77 | Na6(CO3)(SO4)2 |
| C(cr) | -13.98 | 40.5 | 54.48 | C | C(cr) | -16.35 | 39.77 | 56.12 | C |
| C3FH6 | -35.51 | 37.76 | 73.27 | Ca3Fe2(OH)12 | C3FH6 | -28.54 | 46.95 | 75.49 | Ca3Fe2(OH)12 |
| C4FH13 | -47.16 | 48.98 | 96.14 | Ca4Fe2(OH)14:6H2O | C4FH13 | -38.18 | 60.44 | 98.62 | Ca4Fe2(OH)14:6H2O |
| Ca(HPO4)(s) | -1.27 | -0.93 | 0.34 | Ca(HPO4) | Ca(HPO4)(s) | -1.33 | -0.88 | 0.45 | Ca(HPO4) |
| Ca(NO3)2(s) | -14.43 | -8.54 | 5.89 | Ca(NO3)2 | Ca(NO3)2(s) | -16.36 | -10.47 | 5.89 | Ca(NO3)2 |
| Ca(s) | -99.78 | 41.47 | 141.26 | Ca | Ca(s) | -100.86 | 43.98 | 144.84 | Ca |
| Ca2Cl2(OH)2:H2O(s) | -22.23 | 4.3 | 26.53 | Ca2Cl2(OH)2:H2O | Ca2Cl2(OH)2:H2O(s) | -19.64 | 6.89 | 26.53 | Ca2Cl2(OH)2:H2O |
| Ca2Fe2O5(s) | -31.04 | 26.54 | 57.58 | Ca2Fe2O5 | Ca2Fe2O5(s) | -26.19 | 33.45 | 59.64 | Ca2Fe2O5 |
| Ca3(PO4)2(alfa) | -1.07 | 9.37 | 10.44 | Ca3(PO4)2 | Ca3(PO4)2(alfa) | 0.74 | 11.73 | 10.98 | Ca3(PO4)2 |
| Ca4Cl2(OH)6:13H2O(s) | -42.46 | 26.74 | 69.2 | Ca4Cl2(OH)6:13H2O | Ca4Cl2(OH)6:13H2O(s) | -36.51 | 33.87 | 70.38 | Ca4Cl2(OH)6:13H2O |
| Ca4H(PO4)3:2.5H2O(s) | -3.37 | 8.44 | 11.81 | Ca4H(PO4)3:2.5H2O | Ca4H(PO4)3:2.5H2O(s) | -0.97 | 10.84 | 11.81 | Ca4H(PO4)3:2.5H2O |
| CaCl2:2H2O(cr) | -14.95 | -6.93 | 8.03 | CaCl2:2H2O | CaCl2:2H2O(cr) | -14.83 | -6.60 | 8.22 | CaCl2:2H2O |
| CaCl2:4H2O(cr) | -12.3 | -6.93 | 5.37 | CaCl2:4H2O | CaCl2:4H2O(cr) | -12.02 | -6.60 | 5.42 | CaCl2:4H2O |
| CaCl2:H2O(s) | -14.86 | -6.93 | 7.94 | CaCl2:H2O | CaCl2:H2O(s) | -14.77 | -6.60 | 8.17 | CaCl2:H2O |
| CaCO3:H2O(s) | -1.19 | -8.78 | -7.59 | CaCO3:H2O | CaCO3:H2O(s) | -0.15 | -7.71 | -7.56 | CaCO3:H2O |
| CaCrO4(s) | -31.66 | -34.77 | -3.11 | CaCrO4 | CaCrO4(s) | -30.78 | -33.80 | -3.01 | CaCrO4 |
| CaFe2O4(s) | -6.38 | 15.32 | 21.69 | CaFe2O4 | CaFe2O4(s) | -2.88 | 19.96 | 22.84 | CaFe2O4 |
| Calcite | -0.32 | -8.78 | -8.46 | CaCO3 | Calcite | 0.70 | -7.71 | -8.42 | CaCO3 |
| CaMg3(CO3)4(s) | -4.39 | -35.01 | -30.62 | CaMg3(CO3)4 | CaMg3(CO3)4(s) | -1.36 | -31.48 | -30.13 | CaMg3(CO3)4 |
| CaO(cr) | -21.81 | 11.22 | 33.03 | CaO | CaO(cr) | -20.39 | 13.49 | 33.88 | CaO |
| Carnallite | -17.07 | -12.76 | 4.31 | KMgCl3:6H2O | Carnallite | -16.52 | -12.24 | 4.27 | KMgCl3:6H2O |
| Cd(CO3)(s) | 1.68 | -10.43 | -12.1 | Cd(CO3) | Cd(CO3)(s) | -1.13 | -13.24 | -12.11 | Cd(CO3) |
| Cd(cr) | -17.4 | 39.82 | 57.22 | Cd | Cd(cr) | -20.31 | 38.46 | 58.77 | Cd |
| Cd(OH)2(s) | -4.44 | 9.57 | 14.01 | Cd(OH)2 | Cd(OH)2(s) | -6.42 | 7.97 | 14.39 | Cd(OH)2 |
| Cd(SO4)(cr) | -7.81 | -7.88 | -0.07 | Cd(SO4) | Cd(SO4)(cr) | -11.11 | -10.95 | 0.16 | Cd(SO4) |
| Cd(SO4):2.67H2O(cr) | -6.37 | -7.88 | -1.52 | Cd(SO4):2.67H2O | Cd(SO4):2.67H2O(cr) | -9.53 | -10.95 | -1.43 | Cd(SO4):2.67H2O |
| Cd3(PO4)2(s) | -4.9 | 4.43 | 9.33 | Cd3(PO4)2 | Cd3(PO4)2(s) | -15.07 | -4.84 | 10.23 | Cd3(PO4)2 |
| Cd5(PO4)3Cl(cr) | -10.32 | 2.35 | 12.67 | Cd5(PO4)3Cl | Cd5(PO4)3Cl(cr) | -26.00 | -13.33 | 12.67 | Cd5(PO4)3Cl |
| Cd5(PO4)3OH(cr) | -8.41 | 11.43 | 19.84 | Cd5(PO4)3OH | Cd5(PO4)3OH(cr) | -23.12 | -3.28 | 19.84 | Cd5(PO4)3OH |
| CdCl2(s) | -7.94 | -8.57 | -0.63 | CdCl2 | CdCl2(s) | -11.58 | -12.13 | -0.55 | CdCl2 |
| CdCl2:2.5H2O(s) | -6.66 | -8.57 | -1.91 | CdCl2:2.5H2O | CdCl2:2.5H2O(s) | -10.18 | -12.13 | -1.94 | CdCl2:2.5H2O |
| CdCl2:H2O(cr) | -6.89 | -8.57 | -1.68 | CdCl2:H2O | CdCl2:H2O(cr) | -10.48 | -12.13 | -1.64 | CdCl2:H2O |
| CdO(s) | -5.7 | 9.57 | 15.28 | CdO | CdO(s) | -7.76 | 7.97 | 15.73 | CdO |
| CH4(g) | -31.4 | 101 | 132.39 | CH4 | CH4(g) | -35.40 | 100.75 | 136.15 | CH4 |
| Chloroapatite | 5.15 | 10.59 | 5.44 | Ca5Cl(PO4)3 | Chloroapatite | 8.27 | 14.29 | 6.02 | Ca5Cl(PO4)3 |
| Chromite | 10.27 | 25.85 | 15.58 | FeCr2O4 | Chromite | 8.83 | 25.59 | 16.75 | FeCr2O4 |
| Cl2(g) | -51.48 | -48.4 | 3.08 | Cl2 | Cl2(g) | -53.91 | -50.59 | 3.32 |  |
| CO(g) | -18.57 | 10.25 | 28.82 | CO | CO(g) | -20.73 | 9.28 | 30.01 | CO |
| CO2(g) | -1.84 | -20 | -18.16 | CO2 | CO2(g) | -3.03 | -21.21 | -18.18 | CO2 |
| Cr(OH)2(cr) | -15.62 | -4.49 | 11.13 | Cr(OH)2 | Cr(OH)2(cr) | -17.37 | -5.91 | 11.46 | Cr(OH)2 |
| Cr(OH)2(H2PO4)(s) | -4.38 | -3.48 | 0.9 | Cr(OH)2(H2PO4) | Cr(OH)2(H2PO4)(s) | -7.20 | -6.28 | 0.92 | Cr(OH)2(H2PO4) |
| Cr(OH)3(cr) | 0.99 | 8.67 | 7.68 | Cr(OH)3 | Cr(OH)3(cr) | -0.04 | 8.10 | 8.14 | Cr(OH)3 |
| Cr(s) | -45.89 | 44.76 | 90.65 | Cr | Cr(s) | -48.98 | 44.18 | 93.16 | Cr |
| Cr2(SO4)3(s) | -39.9 | -35.04 | 4.86 | Cr2(SO4)3 | Cr2(SO4)3(s) | -46.64 | -40.57 | 6.07 | Cr2(SO4)3 |
| Cr2O3(cr) | 9.24 | 17.33 | 8.09 | Cr2O3 | Cr2O3(cr) | 7.24 | 16.20 | 8.95 | Cr2O3 |
| CrCl2(cr) | -35.54 | -22.63 | 12.91 | CrCl2 | CrCl2(cr) | -39.36 | -26.00 | 13.36 | CrCl2 |
| CrCl3(cr) | -39.08 | -18.55 | 20.53 | CrCl3 | CrCl3(cr) | -43.44 | -22.05 | 21.39 | CrCl3 |
| CrO2(cr) | -7.03 | -15.74 | -8.71 | CrO2 | CrO2(cr) | -8.04 | -16.80 | -8.76 | CrO2 |
| CrO3(cr) | -42.99 | -45.99 | -3.00 | CrO3 | CrO3(cr) | 44.33 | -47.29 | -2.96 | CrO3 |
| CrPO4(green) | -0.42 | -3.48 | -3.06 | CrPO4 | CrPO4(green) | -3.22 | -6.28 | -3.06 | CrPO4 |
| CrPO4(purple) | -6.04 | -3.48 | 2.56 | CrPO4 | CrPO4(purple) | -8.84 | -6.28 | 2.56 | CrPO4 |
| Dolomite | -0.46 | -17.52 | -17.06 | CaMg(CO3)2 | Dolomite | 1.26 | -15.64 | -16.90 | CaMg(CO3)2 |
| Epsonite | -4.31 | -6.2 | -1.9 | Mg(SO4):7H2O | Epsonite | -3.69 | -5.64 | -1.95 | Mg(SO4):7H2O |
| Ettringite-Fe | -36.1 | 19.04 | 55.14 | Ca6Fe2(SO4)3(OH)12:26H2O | Ettringite-Fe | -25.99 | 30.65 | 56.64 | Ca6Fe2(SO4)3(OH)12:26H2O |
| Fe(OH)2(cr) | -4.41 | 8.52 | 12.93 | Fe(OH)2 | Fe(OH)2(cr) | -3.97 | 9.39 | 13.36 | Fe(OH)2 |
| Fe(PO4)(cr) | -3.89 | -10.1 | -6.21 | Fe(PO4) | Fe(PO4)(cr) | -5.02 | -11.14 | 6.13 | Fe(PO4) |
| Fe(s) | -20.72 | 38.77 | 59.49 | Fe | Fe(s) | -21.22 | 39.88 | 61.10 | Fe |
| Fe5(OH)(PO4)3(s) | 408.46 | 6.14 | -402.32 | Fe5(OH)(PO4)3 | Fe5(OH)(PO4)3(s) | 3.83 | -402.32 | 406.15 | Fe5(OH)(PO4)3 |
| FeO(s) | -5.03 | 8.52 | 13.55 | FeO | FeO(s) | -4.61 | 9.39 | 14.00 | FeO |
| Ferrihydrite(am) | -0.49 | 2.05 | 2.54 | Fe(OH)3 | Ferrihydrite(am) | 0.69 | 3.23 | 2.54 | Fe(OH)3 |
| Ferryhydrite | 0.86 | 2.05 | 1.19 | Fe(OH)3 | Ferryhydrite | 2.04 | 3.23 | 1.19 | Fe(OH)3 |
| Gaylussite | -9.23 | -18.71 | -9.48 | CaNa2(CO3)2:5H2O | Gaylussite | -7.20 | -16.82 | -9.62 | CaNa2(CO3)2:5H2O |
| Glaserite | -32.76 | -40.51 | -7.74 | Na2K6(SO4)4 | Glaserite | -27.77 | -35.86 | -8.09 | Na2K6(SO4)4 |
| Glauberite | -15.62 | -13.63 | 1.99 | Na2Ca(SO4)2 | Glauberite | -14.30 | -12.25 | 2.05 | Na2Ca(SO4)2 |
| Goethite | 1.55 | 2.05 | 0.5 | FeOOH | Goethite | 2.47 | 3.23 | 0.76 | FeOOH |
| Gypsum | -1.63 | -6.24 | -4.61 | CaSO4:2H2O | Gypsum | -0.83 | -5.43 | -4.60 | CaSO4:2H2O |
| H2(g) | -13.22 | 30.25 | 43.47 | H2 | H2(g) | -14.20 | 30.49 | 44.69 | H2 |
| H2O(g) | -1.58 | 0 | 1.58 | H2O | H2O(g) | -1.77 | -0.00 | 1.77 | H2O |
| Halite | -5.62 | -4.04 | 1.58 | NaCl | Halite | -5.56 | -4.00 | 1.57 | NaCl |
| HCl(g) | -15.49 | -9.07 | 6.42 | HCl | HCl(g) | -16.79 | -10.05 | 6.74 | HCl |
| Hematite | 4.9 | 4.1 | -0.81 | Fe2O3 | Hematite | 6.74 | 6.47  | -0.27 | Fe2O3 |
| Hexahydrite | -4.57 | -6.2 | -1.63 | Mg(SO4):6H2O | Hexahydrite | -4.03 | -5.64 | -1.61 | Mg(SO4):6H2O |
| Hydrophilite | -18.83 | -6.92 | 11.91 | CaCl2 | Hydrophilite | -18.87 | -6.60  | 12.26 | CaCl2 |
| Hydroxyapatite | 5 | 19.66 | 14.66 | Ca5(OH)(PO4)3 | Hydroxyapatite | 8.90 | 24.33 | 15.44 | Ca5(OH)(PO4)3 |
| K(cr) | -53.33 | 18.33 | 71.66 | K | K(cr) | -53.50 | 19.87 | 73.37 | K |
| K(NO3)(s) | -6.57 | -6.67 | -0.1 | K(NO3) | K(NO3)(s) | -7.26 | -7.36 | -0.10 | K(NO3) |
| K(OH)(s) | -21.39 | 3.21 | 24.6 | K(OH) | K(OH)(s) | -19.98 | 4.62 | 24.60 | K(OH) |
| K-carbonate | -16.61 | -13.58 | 3.03 | K2CO3:1.5H2O | K-carbonate | -15.00 | -11.96 | 3.04 | K2CO3:1.5H2O |
| K-trona | -19.45 | -28.55 | -9.1 | K2NaH(CO3)2:2H2O | K-trona | -18.02 | -27.12 | -9.10 | K2NaH(CO3)2:2H2O |
| K2CO3(cr) | -19.05 | -13.58 | 5.46 | K2CO3 | K2CO3(cr) | -17.57 | -11.96 | 5.60 | K2CO3 |
| K2O(s) | -78.43 | 6.42 | 84.84 | K2O | K2O(s) | -77.46 | 9.24 | 86.71 | K2O |
| Kainite | -11.9 | -12.07 | -0.17 | KMgCl(SO4):3H2O | Kainite | -10.96 | -11.07 | -0.11 | KMgCl(SO4):3H2O |
| Kalicinite | -6.67 | -16.79 | -10.12 | KHCO3 | Kalicinite | -6.31 | -16.59 | -10.27  | KHCO3 |
| KFe(CrO4)2:2H2O(s) | -67.28 | -86.72 | -19.44 | KFe(CrO4)2:2H2O | KFe(CrO4)2:2H2O(s) | -67.17 | -86.72 | -19.56 | KFe(CrO4)2:2H2O |
| KFe3(CrO4)2(OH)6(cr) | -64.22 | -82.62 | -18.4 | KFe3(CrO4)2(OH)6 | KFe3(CrO4)2(OH)6(cr) | -61.85 | -80.25 | -18.40 | KFe3(CrO4)2(OH)6 |
| KH2PO4(cr) | -8.54 | -8.94 | -0.4 | KH2PO4 | KH2PO4(cr) | -9.27 | -9.76 | -0.49 | KH2PO4 |
| Lansfordite | -3.7 | -8.75 | -5.04 | Mg(CO3):5H2O | Lansfordite | -2.87  | -7.92 | -5.06 | Mg(CO3):5H2O |
| Lawrencite | -18.66 | -9.63 | 9.03 | FeCl2 | Lawrencite | -20.10  | -10.70 | 9.39 | FeCl2 |
| Leonhardtite | -5.35 | -6.2 | -0.85 | MgSO4:4H2O | Leonhardtite | -4.90  | -5.64 | -0.74 | MgSO4:4H2O |
| Leonite | -13.24 | -17.24 | -4.01 | K2Mg(SO4)2:4H2O | Leonite | -11.25 | -15.32 | -4.07 | K2Mg(SO4)2:4H2O |
| Lepidocrocite | 1.19 | 2.05 | 0.86 | FeOOH | Lepidocrocite | 2.09  | 3.23 | 1.14 | FeOOH |
| Maghemite(disord) | 0.53 | 4.1 | 3.57 | Fe2O3 | Maghemite(disord) | 2.25 | 6.47 | 4.22 | Fe2O3 |
| Maghemite(ord) | 0.32 | 4.1 | 3.78 | Fe2O3 | Maghemite(ord) | 2.04 | 6.47 | 4.43 | Fe2O3 |
| Magnesite(nat) | 0.12 | -8.74 | -8.87 | MgCO3 | Magnesite(nat) | 0.84 | -7.92 | -8.76 | MgCO3 |
| Magnesite(syn) | -0.69 | -8.74 | -8.05 | Mg(CO3) | Magnesite(syn) | 0.00 | -7.92 | -7.92 | Mg(CO3) |
| Magnetite | 1.83 | 12.61 | 10.78 | Fe3O4 | Magnetite | 4.14 | 15.86 | 11.72 | Fe3O4 |
| Melanterite | -6.7 | -8.94 | -2.25 | FeSO4:7H2O | Melanterite | -7.20 | -9.53 | -2.33 | FeSO4:7H2O |
| Mercallite | -12.85 | -14.25 | -1.4 | KHSO4 | Mercallite | -12.91 | -14.30 | -1.40 | KHSO4 |
| Mg(cr) | -82.55 | 41.51 | 124.06 | Mg | Mg(cr) | -83.54 | 43.77 | 127.31 | Mg |
| Mg(HPO4):3H2O(s) | -2.3 | -0.89 | 1.41 | Mg(HPO4):3H2O | Mg(HPO4):3H2O(s) | -2.50 | -1.09 | 1.41 | Mg(HPO4):3H2O |
| Mg(NO3)2(s) | -24.01 | -8.51 | 15.5 | Mg(NO3)2 | Mg(NO3)2(s) | -26.18 | -10.68 | 15.50 | Mg(NO3)2 |
| Mg(NO3)2:6H2O(s) | -11.09 | -8.51 | 2.58 | Mg(NO3)2:6H2O | Mg(NO3)2:6H2O(s) | -13.26 | -10.68 | 2.58 | Mg(NO3)2:6H2O |
| Mg(SO4)(s) | -15.5 | -6.2 | 9.3 | Mg(SO4) | Mg(SO4)(s) | -15.44 | -5.64 | 9.80 | Mg(SO4) |
| Mg(SO4):H2O(s) | -6.17 | -6.2 | -0.03 | Mg(SO4):H2O | Mg(SO4):H2O(s) | -5.83 | -5.64 | 0.19 | Mg(SO4):H2O |
| Mg-oxychlorur | -12.86 | 13.44 | 26.3 | Mg2Cl(OH)3:4H2O | Mg-oxychlorur | -10.45 | 16.52  | 26.97 | Mg2Cl(OH)3:4H2O |
| Mg3(PO4)2(cr) | -6.72 | 9.47 | 16.19 | Mg3(PO4)2 | Mg3(PO4)2(cr) | -6.02 | 11.10 | 17.12 | Mg3(PO4)2 |
| Mg3(PO4)2:22H2O(s) | -6.54 | 9.46 | 16 | Mg3(PO4)2:22H2O | Mg3(PO4)2:22H2O(s) | -4.91 | 11.09 | 16.00 | Mg3(PO4)2:22H2O |
| Mg3(PO4)2:8H2O(s) | -4.43 | 9.47 | 13.9 | Mg3(PO4)2:8H2O | Mg3(PO4)2:8H2O(s) | -2.81 | 11.09 | 13.90 | Mg3(PO4)2:8H2O |
| Mg5(CO3)4(OH)2:4H2O(s) | -13.82 | -23.72 | -9.91 | Mg5(CO3)4(OH)2:4H2O | Mg5(CO3)4(OH)2:4H2O(s) | -9.53 | -18.41 | -8.88 | Mg5(CO3)4(OH)2:4H2O |
| MgCl2(s) | -29.19 | -6.89 | 22.3 | MgCl2 | MgCl2(s) | -29.81 | -6.81 | 23.00 | MgCl2 |
| MgCl2:2H2O(s) | -19.79 | -6.89 | 12.9 | MgCl2:2H2O | MgCl2:2H2O(s) | -19.71 | -6.81 | 12.90 | MgCl2:2H2O |
| MgCl2:4H2O(s) | -14.33 | -6.89 | 7.44 | MgCl2:4H2O | MgCl2:4H2O(s) | -14.25 | -6.81 | 7.44 | MgCl2:4H2O |
| MgCl2:H2O(s) | -23.11 | -6.89 | 16.22 | MgCl2:H2O | MgCl2:H2O(s) | -23.03 | -6.81 | 16.22 | MgCl2:H2O |
| MgCrO4(s) | 53.01 | -34.73 | -87.74 | MgCrO4 | MgCrO4(s) | 55.65 | -34.01 | -89.65 | MgCrO4 |
| Mirabilite | -6.02 | -7.39 | -1.37 | Na2SO4:10H2O | Mirabilite | -5.11 | -6.82 | -1.71 | Na2SO4:10H2O |
| Monosulfate-Fe | -35.35 | 31.52 | 66.87 | Ca4Fe2(SO4)(OH)12:6H2O | Monosulfate-Fe | -27.44 | 41.51 | 68.95 | Ca4Fe2(SO4)(OH)12:6H2O |
| Na(cr) | -47.88 | 20.16 | 68.04 | Na | Na(cr) | -48.40 | 21.30 | 69.70 | Na |
| Na(NO3)(s) | -5.94 | -4.85 | 1.09 | Na(NO3) | Na(NO3)(s) | -7.02 | -5.93 | 1.09 | Na(NO3) |
| Na2(CO3)(cr) | -11.1 | -9.93 | 1.17 | Na2(CO3) | Na2(CO3)(cr) | -10.38 | -9.10 | 1.28 | Na2(CO3) |
| Na2CO3:7H2O(s) | -9.4 | -9.93 | -0.53 | Na2CO3:7H2O | Na2CO3:7H2O(s) | -8.38 | -9.10 | -0.72 | Na2CO3:7H2O |
| Na2HPO4(cr) | -11.38 | -2.08 | 9.3 | Na2HPO4 | Na2HPO4(cr) | -11.73 | -2.27 | 9.45 | Na2HPO4 |
| Na2O(cr) | -58 | 10.07 | 68.07 | Na2O | Na2O(cr) | -57.49 | 12.10 | 69.60 | Na2O |
| Na3PO4(cr) | -20.75 | 2.96 | 23.7 | Na3PO4 | Na3PO4(cr) | -20.39 | 3.78 | 24.17 | Na3PO4 |
| NaH2PO4(cr) | -9.43 | -7.11 | 2.31 | NaH2PO4 | NaH2PO4(cr) | -10.66 | -8.32 | 2.34 | NaH2PO4 |
| Nahcolite | -4.17 | -14.97 | -10.8 | Na(HCO3) | Nahcolite Na(HCO3) | -4.21 | -15.15 | -10.94 | -10.94 |
| Natron | -8.99 | -9.93 | -0.94 | Na2(CO3):10H2O | Natron | -7.88 | -9.10 | -1.22 | Na2(CO3):10H2O |
| Nesquehonite | -3.68 | -8.74 | -5.06 | Mg(CO3):3H2O | Nesquehonite | -2.96 | -7.92 | -4.96 | Mg(CO3):3H2O |
| O2(g) | -57.62 | -60.5 | -2.88 | O2 | O2(g) | -58.15 | -60.98 | -2.83 | O2 |
| P(cr) | -78.52 | 63.47 | 141.99 | P | P(cr) | -83.89 | 61.85 | 145.74 | P |
| Pentahydrite | -4.95 | -6.2 | -1.26 | MgSO4:5H2O | Pentahydrite | -4.45 | -5.64 | -1.19 | MgSO4:5H2O |
| Periclase | -10.58 | 11.26 | 21.84 | MgO | Periclase | -9.22 | 13.28 | 22.50 | MgO |
| Picromerite | -12.86 | -17.24 | -4.39 | K2Mg(SO4)2:6H2O | Picromerite | -10.79 | -15.32 | -4.53 | K2Mg(SO4)2:6H2O |
| Pirssonite | -9.78 | -18.71 | -8.93 | Na2Ca(CO3)2:2H2O | Pirssonite | -7.85 | -16.82 | -8.97 | Na2Ca(CO3)2:2H2O |
| Polyhalite | -15.98 | -29.72 | -13.74 | K2MgCa2(SO4)4:2H2O | Polyhalite | -12.44 | -26.18 | -13.74 | K2MgCa2(SO4)4:2H2O |
| Portlandite | -11.81 | 11.22 | 23.03 | Ca(OH)2 | Portlandite | -10.11 | 13.49 | 23.60 | Ca(OH)2 |
| Siderite | -0.7 | -11.48 | -10.78 | Fe(CO3) | Siderite | -1.09 | -11.81 | -10.73 | Fe(CO3) |
| Sylvite | -6.7 | -5.86 | 0.84 | KCl | Sylvite | -6.19 | -5.43 | 0.76 | KCl |
| Syngenite | -9.83 | -17.28 | -7.45 | K2Ca(SO4)2:6H2O | Syngenite | -7.66 | -15.11 | -7.45 | K2Ca(SO4)2:6H2O |
| Tachyhydrite | -38.09 | -20.71 | 17.38 | Mg2CaCl6:12H2O | Tachyhydrite | -37.61 | 17.38 | -20.23 | Mg2CaCl6:12H2O |
| Thermonatrite | -10.43 | -9.93 | 0.5 | Na2(CO3):H2O | Thermonatrite | -9.66 | -9.10 | 0.5 | Na2(CO3):H2O |
| Thernardite | -7.03 | -7.39 | -0.36 | Na2SO4 | Thernardite | -6.47 | -6.82 | -0.35 | Na2SO4 |
| Trona | -13.45 | -24.9 | -11.45 | Na3H(CO3)2:2H2O | Trona | -12.64 | -24.26 | -11.62 | Na3H(CO3)2:2H2O |
| Vaterite | -0.9 | -8.78 | -7.87 | CaCO3 | Vaterite | 0.10  | -7.71 | -7.81 | CaCO3 |

## **references**

Abiye, T. A. and Leshomo, J. T. 2013. Groundwater flow and radioactivity in Namaqualand, South Africa. *Environmental Earth Sciences,* 70**,** 281-293.

Erdogan, I., Fosso-Kankeu, E., Ntwampe, S., Waanders, F., Hoth, N. and Rand, A. 2019. Groundwater as an alternative source to irregular surface water in the O'Kiep area, Namaqualand, South Africa. *Physics and Chemistry of the Earth, Parts A/B/C*.

Leshomo, J. 2011. *Investigation of hydrochemistry and uranium radioactivity in the groundwater of Namaqualand, Northern Cape, South Africa*, Johannesburg: MSc thesis, University of Witwatersrand.

Parkhurst, D. L. and Appelo, C. 2013. Description of input and examples for PHREEQC version 3: a computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations. US Geological Survey.

Parkhurst, D. L. and Appelo, C. 1999. User's guide to PHREEQC (Version 2): A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations. *Water-resources investigations report,* 99**,** 312.