## Übungen B (4 ausgewählte Fragen)

Bitte geben Sie die Reaktionsgleichungen der folgenden Reaktionen an. Welche Phase(n) sind unter Standardbedingungen (25 °C, 1 bar) stabil? Wie verlaufen die Gleichgewichtskurven der entsprechenden Reaktionen in Abhängig von Druck und Temperatur? Nutzen Sie die thermodynamischen Daten der beiligen Tabelle 2.2. aus White, W. M. (2007) Geochemistry, John Wiley & Sons, Ltd., S. 52.

1. Albit ↔ Jadeit + Quarz

2. Calcit ↔ Aragonit

3. Andalusit ↔ Sillimanit ↔ Kyanit (Disthen). Als Hilfestellung können Sie in folgende Umwandlungsreaktionen unterteilen:

    a) Andalusit ↔ Kyanit

    b) Sillimanit ↔ Kyanit

    c) Andalusit ↔ Sillimanit

4. Nun liegen diese Berechnungen den thermodynamischen Daten unter Standardbedingungen zugrunde. Wie müsste man vorgehen, um die Gleichgewichte genauer zu berechnen? (Tipp: Rufen Sie sich die Vorgehensweise der Aufgaben 9+10 der Übungen A in Erinnerung.)

where $S_0$ is the entropy at 0 K (configurational, or 'third law' entropy) and $\Delta S_\Phi$ is the entropy change associated with any phase change. Compilations for $S_{298}$ are available for many minerals. Table 2.2 lists some heat capacity constants for the power series formula as well as other thermodynamic data for a few geologically important minerals.

## 2.9 Free Energy

We can now introduce two free energy functions, the Helmholtz Free Energy and the Gibbs Free En-

**Table 2.2: Standard State Thermodynamic Data for Some Important Minerals**

| Phase/ Compound | Formula | $\Delta H^o_f$ (kJ/mol) | S° (J/K-mol) | $\Delta G^o_f$ (kJ/mol) | $\bar{V}$ (cc/mol)* | $C_p$ a | b | c |
|---|---|---|---|---|---|---|---|---|
| $H_2O_g$ | $H_2O$(gas) | -241.81 | 188.74 | -228.57 | 24789.00 | 30.54 | 0.01029 | 0 |
| $H_2O_l$ | $H_2O$(liquid) | -285.84 | 69.92 | -237.18 | 18.10 | 29.75 | 0.03448 | 0 |
| $CO_2$ | $CO_2$ | -393.51 | 213.64 | -394.39 | 24465.10 | 44.22 | 0.00879 | 861904 |
| Calcite | $CaCO_3$ | -1207.30 | 92.68 | -1130.10 | 36.93 | 104.52 | 0.02192 | 2594080 |
| Graphite | C | 0 | 5.740 | | 5.298 | | | |
| Diamond | C | 1.86 | 2.37 | | 3.417 | | | |
| Aragonite | $CaCO_3$ | -1207.21 | 90.21 | -1129.16 | 34.15 | 84.22 | 0.04284 | 1397456 |
| α-Qz | $SiO_2$ | -910.65 | 41.34 | -856.24 | 22.69 | 46.94 | 0.03431 | 1129680 |
| β-Qz | $SiO_2$ | -910.25 | 41.82 | -856.24 | | 60.29 | 0.00812 | 0 |
| Cristobal. | $SiO_2$ | -853.10 | 43.40 | -853.10 | 25.74 | 58.49 | 0.01397 | 1594104 |
| Coesite | $SiO_2$ | -851.62 | 40.38 | -851.62 | 20.64 | 46.02 | 0.00351 | 1129680 |
| Periclase | MgO | -601.66 | 26.94 | -569.38 | 11.25 | 42.59 | 0.00728 | 619232 |
| Magnetite | $Fe_3O_4$ | -1118.17 | 145.73 | -1014.93 | 44.52 | 91.55 | 0.20167 | 0 |
| Spinel | $MgAl_2O_4$ | -2288.01 | 80.63 | -2163.15 | 39.71 | 153.86 | 0.02684 | 4062246 |
| Hem | $Fe_2O_3$ | -827.26 | 87.61 | -745.40 | 30.27 | 98.28 | 0.07782 | 1485320 |
| Corundum | $Al_2O_3$ | -1661.65 | 50.96 | -1568.26 | 25.58 | 11.80 | 0.03506 | 3506192 |
| Kyanite | $Al_2SiO_5$ | -2581.10 | 83.68 | -2426.91 | 44.09 | 173.18 | 0.02853 | 5389871 |
| Andalusite | $Al_2SiO_5$ | -2576.78 | 92.88 | -2429.18 | 51.53 | 172.84 | 0.02633 | 5184855 |
| Sillimanite | $Al_2SiO_5$ | -2573.57 | 96.78 | -2427.10 | 49.90 | 167.46 | 0.03092 | 4884443 |
| Almandine | $Fe_3Al_2Si_3O_{12}$ | -5265.5 | 339.93 | -4941.73 | 115.28 | 408.15 | 0.14075 | 7836623 |
| Grossular | $Ca_3Al_2Si_3O_{12}$ | -6624.93 | 254.68 | -6263.31 | 125.30 | 435.21 | 0.07117 | 11429851 |
| Albite | $NaAlSi_3O_8$ | -3921.02 | 210.04 | -3708.31 | 100.07 | 258.15 | 0.05816 | 6280184 |
| K-feldspar | $KAlSi_3O_8$ | -3971.04 | 213.93 | -3971.4 | 108.87 | 320.57 | 0.01804 | 12528988 |
| Anorthite | $CaAl_2Si_2O_8$ | -4215.60 | 205.43 | -3991.86 | 100.79 | 264.89 | 0.06190 | 7112800 |
| Jadeite | $NaAlSi_2O_6$ | -3011.94 | 133.47 | -2842.80 | 60.44 | 201.67 | 0.04770 | 4966408 |
| Diospide | $CaMgSi_2O_6$ | -3202.34 | 143.09 | -3029.22 | 66.09 | 221.21 | 0.03280 | 6585616 |
| Enstatite | $MgSiO_3$ | -1546.77 | 67.86 | -1459.92 | 31.28 | 102.72 | 0.01983 | 2627552 |
| Forsterite | $Mg_2SiO_4$ | -2175.68 | 95.19 | -2056.70 | 43.79 | 149.83 | 0.02736 | 3564768 |
| Clinozo | $Ca_2Al_3Si_3O_{12}(OH)$ | -68798.42 | 295.56 | -6482.02 | 136.2 | 787.52 | 0.10550 | 11357468 |
| Tremolite | $Ca_2MgSi_8O_{22}(OH)_2$ | -12319.70 | 548.90 | -11590.71 | 272.92 | 188.22 | 0.05729 | 4482200 |
| Chlorite | $MgAl(AlSi_3)O_{10}(OH)_8$ | -8857.38 | 465.26 | -8207.77 | 207.11 | 696.64 | 0.17614 | 15677448 |
| Pargasite | $NaCa_2Mg_4Al_3Si_6O_{22}(OH)_2$ | -12623.40 | 669.44 | -11950.58 | 273.5 | 861.07 | 0.17431 | 21007864 |
| Phlogopite | $KMg_3AlSi_3O_{10}(OH)_2$ | -6226.07 | 287.86 | -5841.65 | 149.66 | 420.95 | 0.01204 | 8995600 |
| Muscovite | $KAl_3Si_3O_{10}(OH)_2$ | -5972.28 | 287.86 | -5591.08 | 140.71 | 408.19 | 0.110374 | 10644096 |
| Gibbsite | $Al(OH)_3$ | -1293.13 | 70.08 | -1155.49 | 31.96 | 36.19 | 0.19079 | 0 |
| Boehmite | AlO(OH) | -983.57 | 48.45 | -908.97 | 19.54 | 60.40 | 0.01757 | 0 |
| Brucite | $Mg(OH)_2$ | -926.30 | 63.14 | -835.32 | 24.63 | 101.03 | 0.01678 | 2556424 |

Data for the standard state of 298.15 K and 0.1 MPa. $\Delta H^o_f$ is the molar heat (enthalpy) of formation from the elements ; S° is the standard state entropy; V is the molar volume; a, b and c are constants for the heat capacity ($C_p$) computed as: $C_p = a + bT - cT^{-2}$ J/K-mol. Modified from Helgeson et al. (1978).
*cc/mol = J/MPa/mol.