Chemical behavior of CO2 in the C-H-O-N system

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Physico-chemical investigation of CO2 fluid in the C-H-O-N system is the most important and effective for improvement of CO2 preservation technique. CO2 should be preserved with the duration of geologic time in natural field of surface of the earth. Liquid CO2 phase is stable within fluid inclusions and frequently is observed under microscopic observation. Liquid CO2 exists surrounding gas bubble of fluid inclusion. The bulk CO2 concentration of a fluid inclusion in which liquid phase is stable is approximately more than a several mole %. In addition, the fluid inclusion more than a several mole % in CO2 concentration contains solid CO2 phase (CO2 hydrate) with liquid CO2 within a fluid inclusion at temperature of 10 degree Celcius below a room temperatures. The following species are examined in the phase relation of C-H-O-N system; CO2, CO, O2, H2O, H2, CH4 and N2. The 7 species are estimated to be in equilibrium at a given temperature and pressure. Here, the following chemical reactions are proposed for the C-H-O system fluid.

CO2=CO+1/2 O2----------(1)

H2O=H2+1/2 O2----------(2)

CH4+2O2=CO2+2H2O ----------(3)

Where, equilibrium constants K(1)-K(3) are given at a given temperature and pressure for equations (1)-(3). In addition, the C-H-O-N system fluid gives the following values of total N=constant, total H =constant, total O=constant and total C=constant in equilibrium condition.

total N=N CO2 + N CO + N H2O + N N2 + N CH4 + N O2 + N N2

total H=2N NH2 + 2N H2O + 4N CH4

total O=N CO + 2N CO2 + N H2O

total C=N CO + N CO2 + N CH4

Where, N CO2 indicates the concentrations of CO2 in mole. total N, total H, total O and total C represent total amounts in moles of chemical species, H-bearing species, O-bearing species and C-bearing species, respectively. Here, quantitative values of 7 species such as CO2, CO, O2, H2O, H2, CH4 and N2 are analyzed based on the 7 equations of K(1), K(2), K(3), total N, total H, total O and total C. The proportion of major species in the earth fluids determined to be controlled strongly by oxygen fugacity.