## **INORGANIC MATERIALS**

## Final Test 100 points

..... name

**1.** a) (10 points) Consider coordination number of cations and anions in the following structure type compounds, fill the blank positions:

n:m = 1:1	CN (a:b)	n:m = 1:2	CN (a:b)	n:m = 1:3	CN (a:b)	n:m = 2:3	CN (a:b)
NaCl		CaF <sub>2</sub>	8:4	ReO <sub>3</sub>		Al <sub>2</sub> O <sub>3</sub>	6:4
CsCl		TiO <sub>2</sub> rutile	6:3	AlCl <sub>3</sub>	6:2	****	****
ZnS		SiO <sub>2</sub> quartz		****	****	****	****
NiAs	6:6	****	****	****	****	****	* * * * *

b) (10 points) Devise a general rule which links stoichiometric coefficients n, m in  $M_n X_m$  with coordination numbers a and b for cations and anions, respectively.

2. (10 points) Zeolite-A (LTA) has a single peak in the <sup>29</sup>Si NMR spectrum (- 89 ppm) and has a Si/Al ratio of 1. Comment on these observations with respect to the Si and Al distribution and ordering.

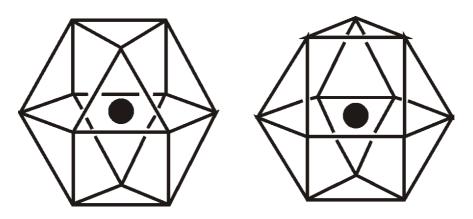
3. (20 points) Semiconductors of the 13/15 and 12/16 types frequently adopt the sphalerite (zinc blende) structure. Draw a unit cell of ZnS-blende and calculate the number of formula units in the unit cell.

4. (10 points) Stishovite is a high-pressure modification of SiO<sub>2</sub> having the rutile structure. Should it have longer or shorter bond lengths then quartz?

**5.** (10 points) Which of these polyhedra represent the coordination environment of a metal atom in

a) copper

b) magnesium



6. The solid state reaction between CaO and SiO<sub>2</sub> is an important process in the cement and iron production (slag formation). Ca<sub>2</sub>SiO<sub>4</sub> is formed in the first step. Write chemical reactions taking place at the interfaces and calculate the Kirkendall ratio for this process

a) (10 points) First, assume counter diffusion of Ca<sup>2+</sup> and Si<sup>4+</sup>

b) (20 points) The assumption a) is unrealistic, because the highly charged Si<sup>4+</sup> is very strongly bound to the oxide network and its diffusion coefficient is negligible. Suggest alternative diffusion process and calculate the Kirkendall ratio.