## MS20-P18 Urea and thiourea: similar compounds – different result

Hanna Tomkowiak[1], Kinga Ostrowska[1], Andrzej Katrusiak[1]

1. Department of Materials Chemistry, Faculty of Chemistry, Adam Mickiewicz University, Umultowska 89b, 61-649 Poznań, Poland

email: hannat@amu.edu.pl

Urea, $(NH_2)_2CO$, and thiourea, $(NH_2)_2CS$, are two of the most common chemical compounds, widely used in chemical practice and industry, mainly for the production of fertilizers, but also pharmaceuticals, insecticides, dyes, plant protection agents, pesticides, corrosion inhibitors, fungicides and as a component explosives.

The single crystals of both compounds have been *in situ* grown from aqueous solution in a diamond-anvil cell [1] and their structure have been determined by X-ray diffraction. Urea and thiourea crystallize as anhydrates at 0.10 MPa. Both these compounds have been intensely studied at normal conditions and in the function of temperature and pressure, while only thiourea hydrates have been obtained from aqueous solution under high pressure.

For urea, three pressure-induced phases: I (tetragonal space group $P\text{-}42_1m$), III (orthorhombic space group $P2_12_12_1$) and IV (orthorhombic space group $P2_12_12$) have been reported with increasing pressure at room temperature; the phase transitions I – III at 0.48 GPa, III – IV at 2.80 GPa. No hydrates have been obtained of urea crystallized at high pressure of aqueous solution. The thermodynamic phase transitions in urea have been rationalized by a microstructural mechanism involving the interplay of pressure-induced molecular reorientations, with hydrogen bonds competing for access to lone-electron pairs of carbonyl oxygen, and by the increasing role of van der Waals interactions [2].

For thiourea, at high-pressure the hydrated or anhydrated crystals can be obtained. Above 0.55 GPa thiourea crystallizes as monohydrate $(NH_2)_2CS{\cdot}H_2O$. At 0.70 GPa another hydrate, $3(NH_2)_2CS{\cdot}2H_2O$, is formed, but above 1.20 GPa anhydrous thiourea becomes stable again. The structural factors favoring the formation of hydrates above 0.55 GPa involve new types of hydrogen bonds involving water molecules and the more efficient molecular packing [3].

**References:**

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## MS20-P19 Study of magnetite, franklinite and gahnite at high pressure and high temperature

Christian Lathe[1], Michael Wehber[1], Hans J. Mueller[1], Joern Lauterjung[1]

1. GFZ German Research Centre for Geosciences, Telegrafenberg, 14473 Potsdam, Germany

email: christian.lathe@gfz-potsdam.de

Magnetite ($FeFe_2O_4$), Franklinite ($ZnFe_2O_4$), and Gahnite ($ZnAl_2O_4$) are Spinels and crystallize in the cubic crystal structure Fd-3m with eight formula units per elementary cell and with the general formula $AB_2O_4$ (where A represents divalent and B trivalent cations, respectively). In the spinel structure, oxygen ions form a cubic-closest packing with 16 octahedral and 8 tetrahedral sites. All three examined Minerals crystallize in the normal spinel structure. This means the tetrahedral sites are occupied by A cations and the octahedral sites are occupied by B cations ($^{[4]}A^{[6]}B_2O_4$).

For the systematic study of the thermo-elastic properties at elevated conditions, Spinels with different iron content are used. The thermal expansion as a function of pressure is deduced from in-situ X-ray diffraction analyses at elevated pressures and temperatures. The interrelation of thermal expansion, compression behavior and iron content is the focus of the study.

The experiments were carried out at HASYLAB (Hamburg, Germany) on two beamlines (F2.1, W2) at DORIS III ring, with a single stage (MAX80) and a double stage (MAX200x) multi-anvil press, respectively. XRD-Spectra at both presses were collected using energy-dispersive mode.

Isothermal experiments were performed at the MAX200x up to 15 GPa at ambient temperature. To obtain the bulk moduli, the data points were fitted to a 3nd order Birch-Murnaghan equation of state yielding to KT = 184(3) GPa and K' = 4.5(2) for Magnetite, KT = 178(3) GPa and K' = 4.6(4) for Franklinite, and KT = 204(4) GPa and K' = 4.9(6) for Gahnite, respectively.

The temperature and pressure dependent volume change were derived from compression experiments using MAX80 apparatus up to 5 GPa at temperatures of 298, 500, 700, 900 and 1100 K.

**Keywords:** Spinel, equation of state, elastic properties, thermal properties