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Molybdenum mobility in magmatic-hydrothermal brines

QIUSHI GUAN[1], DR. YUAN MEI[2], WEIHUA LIU[2] AND JOËL BRUGGER[3]

[1]CSIRO
[2]CSIRO Mineral Resources
[3]Monash University
Presenting Author: Qiushi.guan@csiro.au

Molybdenum (Mo) is a critical metal sourced mostly from magmatic-hydrothermal ore deposits (e.g. Climax-type Mo deposits). Understanding the variability of thermodynamic properties of aqueous Mo complexes under diverse pressures (P) and temperatures (T) is fundamental to understand Mo ore-forming processes. There is a disagreement for Mo(VI) behaviour in experimental studies at T<400˚C. Some studies suggest that Mo(VI) chloride complexes are unlikely to play a significant role in natural fluids, whereas other studies suggest that at magmatic- hydrothermal conditions Mo(VI) is mobilized mainly with chloride complexes.

We applied the *ab initio* molecular dynamic simulations (MD) to investigate the Mo(VI)-Cl complexes and the recent studied $NaHMoO_4$(aq) structure[1]. The simulations reveal that in high-temperature magmatic-hydrothermal fluid conditions, tetrahedral Mo(VI) chloride complex [MoO_2(OH)Cl(aq)] becomes stable. This coordination differs from the octahedral Mo(VI)-chloride complex identified in highly acidic sub-critical fluids (pH<1) at 350 ˚C. The *ab initio* MD was also used to calculate the equilibrium constants of the reaction

$MoO_2(OH)Cl(aq) + H_2O = MoO_2(OH)_2(aq) + HCl(aq)$

Thermodynamic modelling using the data in this study and literature shows that at lower temperatures (350 ˚C, 500 bar), Mo(VI)-Cl^- complex only plays an important role at highly acidic conditions, and $NaHMoO_4$(aq) predominates the solution. However, at higher temperatures (750 ˚C), Mo(VI)-Cl complexes is important in transporting Mo in mildly acidic conditions up to the quartz-muscovite-K-feldspar pH buffer.Our results support that Mo(IV) chloride-complexes could play an important role in the formation of magmatic-hydrothermal Mo deposits.

Reference

1. Shang, L., Williams-Jones, A. E., Wang, X., Timofeev, A., Hu, R., & Bi, X. (2020). *Economic Geology*,*115*(3), 661-669..