

## The Low Velocity High Conductivity layer and abyssal geological process for abiogenetic gas in Songliao basin

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### The Low Velocity High Conductivity (LVHC) layer nature and abyssal geological process

A commercial abiogenetic gas field [1,2] was found around Xujia fault depression, which has a volume of about  $500 \times 10^8 \text{ m}^3$ , in Songliao basin. The LVHC layer underneath and the relevant abyssal geological processes may be related to the formation of abiogenetic gas. In this paper, we discuss the nature of the LVHC layer and abyssal geological processes in relation to the formation mechanics of abiogenetic gas.

In Songliao basin, mantle uplift [3] and many Moho boundary breaks were observed in deep reflection seismic profiles. More thermal diapirs developed under the fault depression. Magmatic activities were intense. Deep major faults cut even to Moho forming upwelling mantle fluid a channel and a material interchange geological space.

Lithosphere horizontal motion made high heat mantle fluid form flat LVHC layers at weak geological space in upper and bottom of midcrust. We inferred its fluid nature by comparing deep reflection seismic polyspectrum characteristics in combination with seismic wave propagation theories with reflected amplitude analysis. Widespread high heat geothermal value and high conductivity indicate that it may be abundant in metal elements. All are the results of intricate abyssal geological processes [4] which are very favorable for Fischer-Tropsch synthesis.

### Conclusion

The LVHC layer is metal-rich high heat mantle fluid which is closely related to the formation of abiogenetic gas. The complicated abyssal geological process provided necessary conditions for Fischer-Tropsch synthesis to happen.

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## Structure and energetics of the orientational ordering of carbonate in vaterite calcium carbonate by molecular modeling

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Vaterite is the least stable phase of anhydrous crystalline calcium carbonates, a rare mineral in geological setting. But it may be an important precursor in several carbonate-forming processes and plays an important role in biological processes. However, issues such as vaterite crystal nucleation, transformation, and stabilization in host materials remain largely unresolved. Understanding these issues may lead to answers to some of fundamental questions including carbonate formation in geological systems and occurrence of vaterite in biogenic systems. All of the above require a basic knowledge of the crystal structure of vaterite and its order-disorder transition. Molecular modeling is employed to understand the crystal structure and orientational order of  $\text{CO}_3$  in vaterite. By applying a temperature-annealing to the molecular dynamics simulations, a more stable structure with fully ordered  $\text{CO}_3$  is found. The space group of this newly-derived vaterite structure [1] is  $P6_322$  (#179) with  $z=18$  and cell dimensions of  $\sqrt{3}$  times in  $a$ , and 3 times in  $c$  of the previous well-accepted suggested disordered structure [2]. This structural ordering has been confirmed by new microscopic observations. Additional molecular dynamics simulations are employed to understand the thermodynamics and kinetics of the orientational ordering of  $\text{CO}_3$  in vaterite. Along the [001] direction, the simulation results suggest possible stacking disorder in vaterite. Cyclic high-temperature simulated-annealing MD simulations show that the  $\text{CO}_3$  orientational disorder-order transition is thermally activated. The potential energy change from disordered to ordered vaterite is  $-10.6 \text{ kJ/mol}$ . The kinetic barrier for the transition is  $93.9 \pm 9.6 \text{ kJ/mol}$  with a pre-exponential factor of  $\sim 1.6 \times 10^{13} \text{ s}^{-1}$ . The heat capacity is estimated to be  $102.1 \pm 0.4 \text{ J/K/mol}$ , comparable to an experimental result  $91.5 \pm 3.8 \text{ J/K/mol}$ . A good linear fit of logarithm transition rate to inverse temperature indicates that the transition is controlled by a single activation process that is related to the librational motion of  $\text{CO}_3$  in vaterite.

[1] Wang & Becker (2009) *American Mineralogist* **94**, 380–386. [2] Kamhi (1963) *Acta Crystallographica* **16**, 770–772.