The ore-forming mechanism of the No. 6 lithium-enriched coal seam from the Ganbanwusu Mine, Inner Mongolia, China: DFT calculations and ICP-MS determinations of Li isotopes

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Comprehensive utilization of trace elements including Li, U enriched in coals will probably twist the decline trend of the whole coal economy. Clarifying their sources and the formation modes will promote further exploration of available resources. In the present work, a novel ore-forming mechanism of the No. 6 lithium-enriched coal seam from the Ganbanwusu Mine, Inner Mongolia, China was suggested in which released Li from the moyite of Yinshan old land was brought into the peat by small carboxylate and in subsequent coalification, this fraction of Li was released into the pore water and was adsorbed by kaolinite edge sites (octahedral layers and/or tetrahedral layers). DFT calculations and ICP-MS determinations confirmed our speculations. The adsorption of Li on numerous available octahedral layer sites of fine kaolinite particles scattered into coals determined the δ^7Li of the No. 6 coal seam. Specifically, we figured out $\Delta^{7/6}Li_{organolithium\text{-}aq}$ = -0.35‰ (chelation), $\Delta^{7/6}Li_{octahedral\ layer\text{-}aq}$ = 4.36‰ and $\Delta^{7/6}Li_{tetrahedral\ layer\text{-}aq}$ = -4.53‰ (adsorption). The No. 6 coal seam δ^7Li 7.38‰ was calculated based on the moyite δ^7Li 3.37±0.13‰, in excellent agreement with δ^7Li 7.04±0.93‰ determined. However, the relative decrease of available octahedral layer site of the partings resulted in the enhancing of adsorption of Li on tetrahedral layer sites and negative deviation of the partings δ^7Li to 5.07±0.22‰.