

Supplementary materials:
Ultra-fine mineral associations in superhigh-organic-sulfur Kentucky
coals

James C. Hower,^{a,*} Debora Berti,^b Michael F. Hochella, Jr.^{c-d}

^a University of Kentucky, Center for Applied Energy Research, 2540 Research Park Dr.,
Lexington, Kentucky 40511 USA (Hower: 1-859-257-0261; james.hower@uky.edu)

^b National Center for Earth and Environmental Nanotechnology (NanoEarth), Virginia Tech,
1991 Kraft Drive, Blacksburg, Virginia 24061 USA¹

^c Department of Geosciences, Derring Hall, Virginia Tech, Blacksburg, Virginia 24061 USA

^d Subsurface Science and Technology Group, Energy and Environment Directorate, Pacific
Northwest National Laboratory, Richland, WA 99352 USA

*Corresponding author

¹ now at: Department of Geology & Geophysics, Texas A&M University, College Station, TX 77843-3115

Supplementary materials

Powder X-ray Diffraction

Both samples show the presence of pyrite and sulfates, specifically melanterite and szomolnokite that are two soluble ferrous sulfates forming from weathering of pyrite (Jambor et al., 2000). Melanterite is usually the first mineral to form on the oxidized rim of sulfides (Nordstrom, 1982).

A diffuse, broad reflection centered around $23^\circ 2\theta$, caused by the presence of amorphous is more pronounced in sample 71205, reflecting a higher amorphous content but also less crystalline phases in the mineral fraction (Supplementary Figure). Besides the sulfides and sulfates reported above, only mica (illite) and kaolinite can be positively identified, though the presence of gibbsite, mixed-layer clays, and zeolite is suggested. In sample 5400, a few intense, narrow peaks are present in the low-angle region of the pattern that cannot be assigned to clay minerals (2-theta angle too far or missing of higher-order peaks). These peaks are attributed to copiapite a hydrate Fe^{2+} , Fe^{3+} sulfate, and alunogen, a hydrated Fe^{3+} aluminum sulfate that is known to form from acid sulfate weathering (Jambor et al., 2000). Melanterite, szomolnokite, copiapite, and alunogen are common minerals in coal deposits (Jambor et al., 2000). Finally, the XRD peak at $\sim 9.5^\circ 2\theta$ cannot be fully explained by copiapite and indicates the presence of zeolite, most likely melanterite.

Jambor, L.J., Nordstrom, D.K., Alpers, C.N., 2000. Metal-sulfate salts from sulfide mineral oxidation. *Reviews in Mineralogy and Geochemistry* 40, 303-350

Nordstrom, D.K., 1982. The effect of sulfate on aluminum concentration in natural waters: Some stability relations in the system $\text{Al}_2\text{O}_3\text{-SO}_3\text{-H}_2\text{O}$ at 298K. *Geochim. Cosmochim. Acta* 46, 681-692.

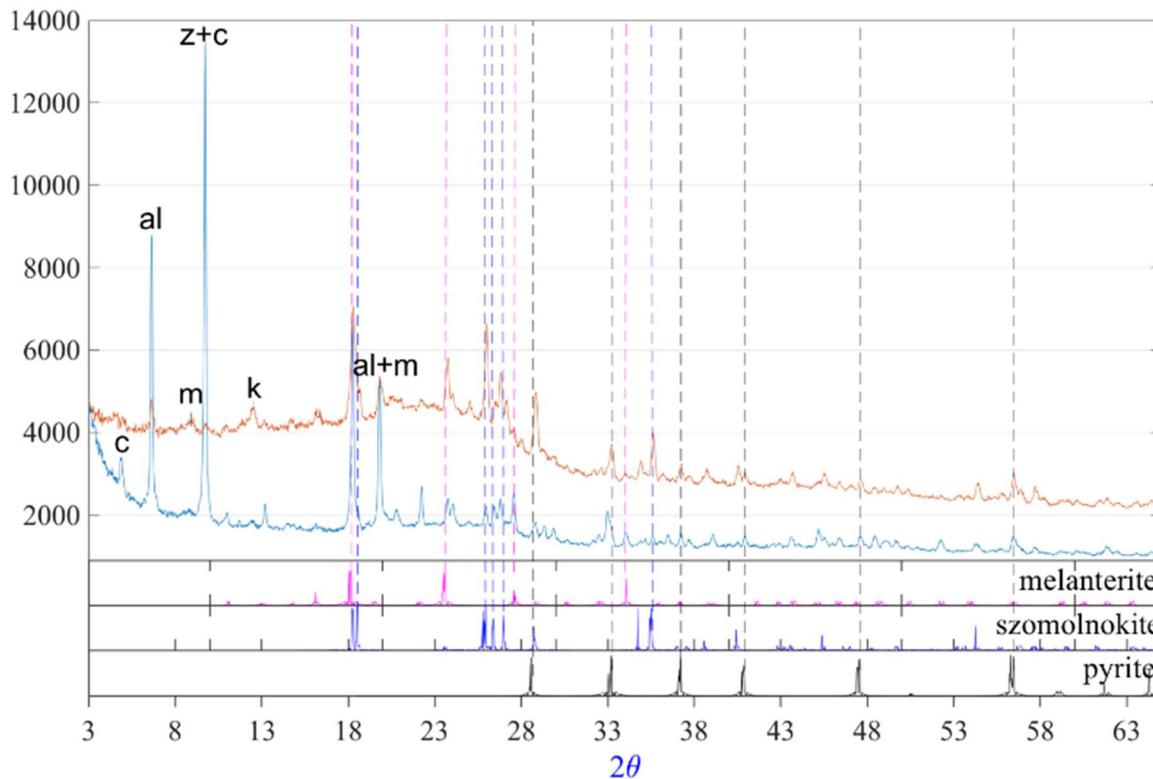


Figure S1. Powder X-ray diffraction pattern of samples 71205 (red) and 5400 (blue). Simulated XRD patterns of melanterite (pdf 04-010-6331), szomolnokite (pdf 04-016-5074), and pyrite (pdf 00-042-1340) are plotted for easy comparison of peak positions. Other minerals identified in sample 71205 are mica (m) and kaolinite (k) and, in sample 5400, alunogen (al), copiapite (c), and melanterite (z). Peaks of clays are present in sample 5400 but their intensity is too low above the background for positive identification. Gibbsite and quartz (not marked) are likely present but their peaks are too weak for positive identification. Coal is responsible for the diffuse reflection centered around $23^\circ 2\theta$.