Mineral properties identified as most influential drivers of mineral-associated organic carbon formation using a community-based sorption database

Authors: Maria E. Macfarlane[1], Haruko M. Wainwright[1,2]*, Jon K. Golla[3], Katerina Georgiou[4], César Terrer[1], Jennifer Pett-Ridge[5,6,7], Mavrik Zavarin[3]

Affiliations
[1]Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA
[2]Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA
[3]Seaborg Institute, Lawrence Livermore National Laboratory, Livermore, CA, USA
[4]Physical Department, Oregon State University, Portland, OR, USA
[5]Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, CA, USA
[6]Life and Environmental Sciences Department, University of California Merced, Merced, CA, USA
[7]Innovative Genomics Institute, University of California, Berkeley, CA USA

*Corresponding author: hmwainw@mit.edu

Abstract

Increasing soil organic carbon (SOC) storage has the potential to substantially offset anthropogenic CO_2 emissions. Globally, mineral-associated organic carbon (MAOC) constitutes the majority of SOC (~65%) and represents a more persistent SOC pool for sequestration. However, the factors controlling how much organic carbon sorbs to soil minerals remain poorly understood, limiting our ability to predict and optimize SOC sequestration strategies. Here, we compiled a first-of-its-kind community database with sorption experiments of organic compounds on a range of soil minerals (1,673 data points). We found a general, negative pH dependency of the partition coefficient K_d (reflecting the amount of mineral-sorbed organic carbon) across anionic compounds, while the cationic compound showed a positive pH relationship with the partition coefficient. In addition, iron oxides and extracellular polymeric substances had the highest K_d values. Our random forest model reproduces the observed K_d ($R^2 = 0.77$, $RMSE = 0.59$) and points to mineral type and surface area characteristics as the dominant drivers of MAOC sorption phenomena, as opposed to the minor role of organic compound properties. Our analysis suggests that incorporating more mineral-specific parameters in soil carbon cycling models could inform and improve predictions of MAOC, and in turn, the effectiveness of SOC management strategies.

Keywords: *soil, data-driven prediction, long-term carbon storage*

Synopsis: Soil carbon only mitigates CO_2 emissions if it remains belowground long term. We used a data-driven strategy to analyze organic-compound-specific sorption experiments and identified mineral properties as key drivers of long-term soil carbon storage.

Introduction

Globally, soils hold the largest terrestrial carbon pool, containing roughly 1,277–1,425 Gt of organic carbon in the top meter (Jackson et al. 2017). Because of soil's carbon storage capacity and additional sink potential, increasing soil organic carbon (SOC) has been proposed as a long-term carbon dioxide removal (CDR) strategy (Minasny et al. 2017; Bossio et al. 2020). In fact, it is estimated that the protection and restoration of SOC could capture up to 1.5 Gt C yearly (Bossio et al. 2020). However, not all SOC remains in the soil over timescales relevant to effectively mitigate atmospheric CO_2 levels (Hemingway et al. 2019). SOC is often described as having three functionally distinct components: dissolved organic carbon (DOC), particulate organic carbon (POC), and mineral-associated organic carbon (MAOC) (von Lützow et al. 2007; Lavallee et al. 2020). DOC (operationally defined as <0.45 μm) is the most mobile and transient pool of SOC (Guo et al. 2024). POC is defined as partially decomposed plant material, while MAOC consists of, low-molecular-weight carbon compounds that are either physically or chemically bound to mineral surfaces (Lavallee et al. 2020).

While physical protection of MAOC via aggregate formation or via spatial inaccessibility can be an important SOC stabilization mechanism (Egli et al. 2008; Rowley et al. 2018), here, we focus on MAOC that is chemically bound to minerals, encompassed by the term "sorption". Sorption processes can include van der Waals bonds, hydrophobic interactions, cation exchange and bridging, as well as ligand exchange (Kleber et al. 2021). Through these mineral associations, MAOC is better protected from microbial degradation than POC (Lalonde et al. 2012; Gentsch et al. 2018), and thus exhibits longer turnover times (averaging 129 years for MAOC compared to 23 years for POC; Grant et al. 2022; Sokol et al. 2019; Zhou et al. 2024). Increasing this more persistent pool of SOC will require increasing C inputs, efficiency of MAOC formation (e.g., via pH or plant and microbial traits that affect organic compound composition and chemistry), or the availability of reactive mineral surfaces. (Slessarev et al. 2022; Buss et al. 2024; Tao and Houlton 2024).

Previous research has identified five drivers that promote MAOC formation via sorption processes: water, vegetation, microbiota, pH, and reactive soil-mineral surfaces (Kleber et al. 2015; Sokol et al. 2022). Many aspects of these drivers have been investigated, such as soil moisture (Lacroix et al. 2022; Heckman et al. 2023), above- and belowground carbon input (Sokol 2019), plant exudates (Keiluweit et al. 2015; Li et al. 2021; Shabtai et al. 2024), and microbial biomass and necromass (Liang et al. 2017; Wang et al. 2021). The favorable effect of low pH on MAOC formation can be ascribed to variably charged surfaces of minerals carrying hydroxyl groups that are protonated in acidic conditions, thereby promoting the retention of organic compounds through ligand exchange (Kleber et al. 2021). Perhaps the most intuitive driver of MAOC is the amount of available mineral surface area, which is strongly dependent on a soil's underlying parent material and weathering rates (Kleber et al. 2015; Georgiou et al. 2022; Slessarev et al. 2022). These five drivers interact with each other, which makes it difficult to individually parse their influence on MAOC formation. Hence, there is a need to constrain such investigations at a fundamental level to distinguish first-order controls.

Given a fixed amount of mineral surface area, the extent and mechanisms of MAOC formation are influenced by characteristics of the organic carbon compounds and minerals involved. For organic compounds, molecular weight and functional groups affect potential interaction mechanisms with minerals and their pH sensitivity (Keiluweit and Kleber 2009; Kleber et al. 2021). Organic compounds that exhibit little variety in functional groups will have fewer ways to form mineral associations than more complex moieties that include nitrogen (N) and phosphorus (P). Recent work has indicated that organic molecules containing N and P may be more likely to be adsorbed as MAOC due to their high affinity to mineral surfaces (Spohn 2024). Furthermore, amphiphilic organic compounds may form hydrophobic clusters in addition to direct sorption to the mineral surface, resulting in multilayer sorption (Kleber et al. 2007; Gao et al. 2020; Underwood et al. 2024). For minerals, surface chemistry, mineral surface area, and mineral composition determine sorption capacity and affinity for MAOC formation (Baldock and Skjemstad 2000; Kleber et al. 2015). The surface chemistry of minerals, such as their surface charge and acidity constants, affects the mechanisms through which SOC can be bound. The surface acidity constants (pKa) of minerals determine their affinity for attracting organic molecules, since pKa is a measure of whether their functional groups are protonated and the net charge on the surface. Finally, the mineral type incorporates a unique arrangement of elements and functional groups, which allows for mineral-specific interactions with organic compounds. All these characteristics influence the extent of MAOC formation via sorption processes.

Systematic knowledge is lacking to identify and predict the specific organo-mineral combinations that allow greater MAOC formation. Although many studies have investigated MAOC formation using sorption experiments, most are limited in the number of data points and parameter ranges, constraining their broad applicability. The most comprehensive study to date compiled 402 observations from DOC sorption experiments on soils from six soil orders (Abramoff et al. 2021). Abramoff et al. found that the amount of organic carbon, pH, soil order, and climate conditions were the most influential variables in the estimation of the partition coefficient K_d, a measure of the amount of organic carbon sorbed to the mineral (Abramoff et al. 2021). However, they did not include key parameters influencing MAOC formation, such as mineral surface area or pKa. Furthermore, they focused broadly on DOC, which can include a wide range of organic molecules, thus rendering difficult the distinction of MAOC drivers influenced by carbon source or mineral composition (Jagadamma et al. 2012; Newcomb et al. 2017). To our knowledge, no study to date has investigated the drivers of chemical association between organic carbon and minerals vis-à-vis MAOC using comprehensive organic-compound- and mineral-specific sorption data.

The objective of our study is to improve our predictive understanding of soil carbon persistence and sequestration potential in soil. We have leveraged a recently developed database of sorption experiments (Zavarin et al. 2022), to which we have added data on organic-compound-specific sorption on a broad range of soil minerals. By expanding and analyzing this comprehensive database, we aim to identify drivers controlling MAOC formation via sorption processes. We then use a Random Forest regression to predict organic-compound-specific sorption on soil minerals, and identify the most important parameters for the formation of mineral associations. Our analysis lays the groundwork for a community sorption database strategy that can help inform MAOC models by testing the suitability of parameters available at the global scale and improving the prediction of MAOC, and in turn, the effectiveness of managing SOC accrual as a climate mitigation strategy.

Materials and Methods

Data Acquisition and Transformations

We used and expanded the Lawrence Livermore National Laboratory-Surface Complexation/Ion Exchange (L-SCIE) database, which is a collection of adsorption experiments and their metadata in a findable, accessible, interoperable, and reusable (FAIR) format (Zavarin et al. 2022). Prior to our work, the L-SCIE database only partially comprised sorption data for organic compounds or classes found in soil, focusing to a greater extent on radionuclide sorption (Chang et al. 2023). For our current study, we mined the literature for additional sorption experiments with organic compounds such as humic acid (HA), fulvic acid (FA), and more complex compounds such as extracellular polymeric substances (EPS), to fill these data gaps. We searched specifically for mineral-organic-compound pairs that were underrepresented in the L-SCIE database and for organic compounds that are more complex to represent soil conditions more appropriately. Papers had to include sorption data across a range of pH (sorption experiments with measurements at only one pH value were excluded), had to record the initial concentration of organic compound added, the amount sorbed, the mineral concentration, and the kind and amount of electrolytes added to solution to allow for the calculation of ionic strength. PlotDigitizer was used to extract data points from plots. We acquired a total of 1,673 sorption data points and experimental conditions (e.g., background electrolyte concentration, mineral surface area, gas composition, etc.). These data were unified by the L-SCIE Surface Complexation Database Converter code, which performs unit conversions and propagated error conversions (Zavarin et al. 2022). Once converted and filtered for the mineral types and organic compounds of interest, the output of this code is a .csv file that was used for further data analysis in R (L-SCIE database can be found here: https://github.com/mzavarin/L-SCIE). To account for intrinsic measurement and extrinsic digitization errors, we excluded data with sorption values greater than 99% and lower than 1%. We separated our analysis in (1) a broader overview of the database, including all organic compounds, and (2) a more targeted analysis on only organic compounds naturally occurring in soil (i.e., HA, FA, ketogluconate, and oxalic acid), for which we performed a principal component analysis (described in Materials and Methods: Exploratory Data Analysis) and a random forest regression (described in Materials and Methods: Predictive Modeling).

Organic compounds were characterized by their molecular weight, except for the more complex organic compounds for which no molecular weight was reported (Table S1). This was especially important for characterizing HA and FA, since they are operationally defined and do not represent distinct SOC compounds (Kelleher and Simpson 2006). HA and FA are classes of compounds that have been studied historically, although their nature has been subject of debate in soil literature (Sutton and Sposito 2005; Schmidt et al. 2011). We refined molecular weight estimates for HA and FA by collecting information directly from the original manuscripts, if it was reported, or from additional literature on the specific soil or source of the compounds (Perminova et al. 2003). The molecular weight of a compound has been shown to influence its sorption behavior on soil minerals and therefore, it was deemed appropriate to translate the organic compounds to numerical terms (Kleber et al. 2015).

We focused our literature search on 1:1-layer and 2:1-layer phyllosilicates, aluminum (Al) and iron (Fe) oxides, and quartz to cover the most abundant soil minerals (Ito and Wagai 2017). We grouped bentonite, montmorillonite, and smectite together using the term smectite, given that smectite as a mineral class includes all three minerals. The majority of studies in our database measured the specific surface area of each mineral used. If only the mineral's particle size was given, we converted it based on the source material to unify the surface areas to m^2/g. The unified values are summarized as mean ± standard deviation across the collected experiments in Table 1.

Table 1: Mineral types, mean specific surface area [m^2/g] ± standard deviation, and surface acidity constant pKa (the surface protonation constant) of minerals used in the assembled experiments. pKa's of smectite: 10.5, 8.3, and 5.8 for publications reporting smectite, montmorillonite, and bentonite, respectively.

Mineral	Mean specific surface area	pKa	Mineral	Mean specific surface area	pKa
ferrihydrite	490.0 ± 149.3	7.3	hematite	19.5 ± 17.6	7.4
boehmite	130.3 ± 63.2	6.9	kaolinite	18.2 ± 9.6	6.5
smectite	73.6 ± 57.0	10.5, 8.3, 5.8	vermiculite	12.9	6.4
goethite	70.4 ± 24.2	7.1	alumina	7.1 ± 6.3	7.5
gibbsite	23.8 ± 28.7	8.3	quartz	4.1 ± 7.9	4.8

The surface acidity constants of minerals (pKa) were taken from the RES^{3}T database (Brendler et al. 2003). This database contains digitized mineral-specific thermodynamic sorption data, including acidity constants. We selected the protonation constants, pK1, derived from a diffuse double layer model to represent mineral pKa and ensure comparability across all minerals (Table 1).

Prior to data analysis, we transformed the collected parameters to obtain ionic strength and the partition coefficient K_d. Ionic strength, a measure of the charge of ions in solution, was calculated according to:

$$I = \frac{1}{2} \sum c_i z_i^2 \tag{1}$$

where c_i is the ion concentration and z_i is the charge of ion. The partition coefficient K_d describes the ratio of the amount of sorbate that is adsorbed to the mineral surface, divided by the remaining amount in solution after reaching equilibrium:

$$K_d = \frac{\frac{c_{Sorbate\,(sorbed)}}{c_{Mineral}}}{c_{Sorbate\,(aqueous)}} \tag{2}$$

where we define $c_{Sorbate\,(sorbed)}$ as the equilibrium concentration of organic compound that is sorbed to the mineral, $c_{Mineral}$ as the amount of mineral added to the experiment, and $c_{Sorbate\,(aqueous)}$ as the concentration of organic compound that stays in solution after reaching equilibrium. As such, K_d was standardized for the added mineral concentration and has units of [L/g]. We further log-transformed K_d to normalize its distribution for statistical purposes. To compare log(K_d) across mineral types, we first evaluated homoscedasticity with the Levene's test, then used a one-way analysis of variance (ANOVA), followed by Tukey's Honestly Significant Difference (HSD) post-hoc test ($\alpha = 0.05$) to identify pairwise differences.

Exploratory Data Analysis

We first investigated the relationship among the collected parameters by conducting a principal component analysis (PCA). To consider a variable important in contributing to a principal component, we required its loading to be higher than 0.6. The numerical predictor variables were standardized as a z-score, by centering the data and scaling to unit variance to allow comparability. The PCA was based on a correlation matrix and conducted with the R package *stats* (R Core Team 2023). Next, we performed a correlation analysis with the R package *corrplot* (R Core Team 2023), for which we used three significance levels (0.001, 0.01, and 0.05).

Predictive Modeling

We chose random forest (RF) algorithms to predict the target variable log(K_d), since previous sorption modeling studies have used RF to accommodate nonlinear relationships (Abramoff et al. 2021; Chang et al. 2023). In addition, RF algorithms have a lower risk of overfitting compared to other machine-learning models (Breiman 2001). Predictor variables included: specific surface area of minerals ($SSA_{Mineral}$), the initial concentration of the sorbate ($Initial\ conc._{Org.compound}$), molecular weight of the organic compounds ($MW_{Org.compound}$), the type of mineral, the surface acidity constant of each mineral ($pKa_{Mineral}$), ionic strength (I), and pH.

Prior to modeling, we scaled all numerical predictor variables (min-max normalization) to ensure comparability among variables in the model. We built our random forest model according to Breiman and Cutler's Fortran code for RF regressions, using the R package *RandomForest* (Breiman et al. 2002, R Core Team 2023). To account for the dependency of observations within experiments, we cross-validated the model with an adapted leave-one-out method, namely a "leave-one-experiment-out cross validation". Iterating through all experiments, only one experiment and its observations were taken as test data, while the rest of the dataset was used as a training set, until all experiments were used once as test data, on which we tested the prediction accuracy of our model. We restricted the number of trees to 1000 and the maximum number of independent variables used at each split to a third of the total number of predictors, to ensure optimal utilization of information contained across predictor variables (Boulesteix et al. 2012). We evaluated model performance with R^2 and the root mean squared error ($RMSE$).

The variable importance was calculated based on the %-increase in MSE upon permutation of a variable. This permutation-based measure computes the MSE for every regression tree using the test data, permutes each predictor variable, and calculates the differences in MSE of the model with and without the permuted variable (Breiman et al. 2002; Grömping 2009). To improve the comparison among predictor variables, the variable importance scores were normalized on a scale of 0 to 100%, to indicate their relative importance towards the model outcome.

Geochemical Modeling

We complemented our data analysis with geochemical simulations to investigate the influence of mineral solubility and aqueous associations between organic compounds and metals (with a known strong pH dependence) on the resulting K_d values from our database compilation. These effects can compound with each other and cause a non-monotonic relationship between pH and K_d (described further in Results and Discussion). We used the open-source code Reaktoro (version 2.13, Leal 2015) to interrogate the behavior of ferrihydrite and alumina in the presence of the common root exudate oxalic acid through a set of 0-D batch reactor simulations.

We derived thermodynamic constants describing mineral solubility and the degree of aqueous complexation between the oxalate ion ($C_2O_4^{2-}$; herein denoted as Ox^{2-} for simplicity) and ferric iron (Fe^{3+}) or the aluminum ion (Al^{3+}) from ThermoChimie version 12a (Madé et al. 2025). We specified $Fe(OH)_4^-$, $Fe(OH)^{2+}$, $Fe_2(OH)_2^{4+}$, $Fe(Ox)^+$, $Fe(Ox)_2^-$, and $Fe(Ox)_3^{3-}$ as aqueous complexes in the Fe-Ox system and $Al(OH)^{2+}$, $Al(OH)_2^+$, $Al(OH)_{3(aq)}$, $Al(OH)_4^-$, $Al(HOx)^{2+}$, $Al(Ox)^+$, $Al(Ox)_2^-$, $Al(Ox)_3^{3-}$, $Al_2(Ox)_4(OH)_2^{4-}$, $Al_3(Ox)_3(OH)_3$, and $Al_4(Ox)_4(OH)_4$ for the Al-Ox system. The activity coefficients of aqueous species were calculated using the extended Debye-Hückel equation. All simulations were conducted at standard temperature and pressure. The concentration of dissolved iron and aluminum were set to be in equilibrium with a fixed amount of ferrihydrite and alumina, respectively. We varied the concentration of oxalic acid to represent a case where the chemical species is virtually absent in the system versus a case that mimics experimental conditions. Equilibrium pH was varied from 2 to 10 to encapsulate the range of values described in the sorption experiments we surveyed. Under this combination of conditions, reactions proceed until Gibbs free energy is minimized and thus chemical equilibrium is reached.

Results and Discussion

Organic-compound-specific Sorption Database Overview

To evaluate the factors controlling mineral-associated organic carbon formation, we compiled a community database of 1,673 sorption experiments from 28 publications and analyzed the relationships between mineral characteristics, organic compound properties, and the partition coefficient (K_d). The current database includes eleven different organic compounds (Figure 1a), ranging from simple compounds (e.g., oxalic acid) to more complex compound classes, such as extracellular polymeric substances (EPS) which are released by soil microorganisms for nutrient acquisition, protection, and to maintain osmotic potential (Zhang et al. 2024). Hereafter, we will for simplicity refer to both organic compounds and compound classes as organic compounds. These compounds have a variety of organic moieties and functional groups, representing molecules affiliated with soil mineral-associated carbon as well as some contaminants (Whalen et al. 2022). The database also contains ten minerals, including some of the most abundant soil minerals (Ito and Wagai 2017). Across all the carbon compounds, the majority of data points were available for goethite (*n*=658) and kaolinite (*n*=406), which are both widely found in soil.

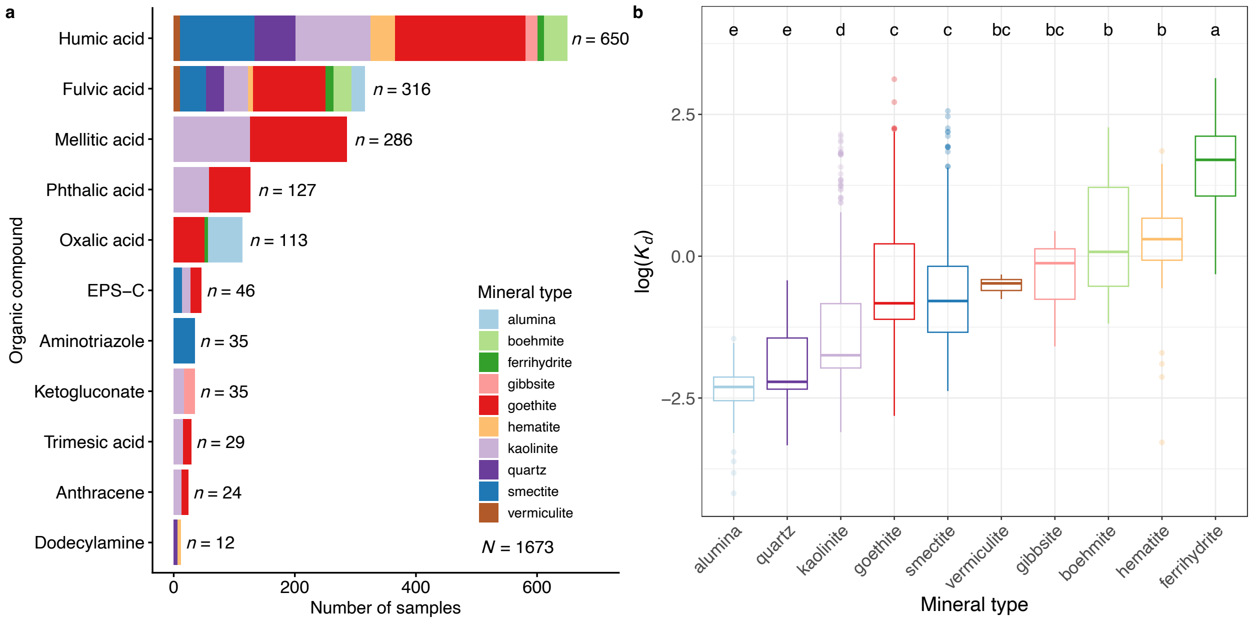

Figure 1: Overview of organic-compound-specific sorption data (N = 1673) for ten soil minerals, collected from 28 publications. a) Number of data points per mineral type for each organic compound. EPS-C = Carbon in extracellular polymeric substances. n equals the number of data points. b) Variation and magnitude of log(K_d) (a measure of the amount of organic compound sorbed to the mineral, standardized by mineral concentration) across mineral types. Boxplots show the median, interquartile range (box), and values within 1.5 times the interquartile range (whiskers); points outside this range are plotted as outliers. Different letters above the boxplots indicate significant differences.

Minerals with low surface area tended to have lower log(K_d) values, while ferrihydrite, a mineral with a large surface area, exhibited the highest values (Figure 1b). However, the wide ranges of log(K_d) within mineral types highlighted that the sorption magnitude also depends on the specific organic compound. For example, the range extended more than four orders of magnitude for goethite and kaolinite, which included the largest number of organic compounds across the experiments.

The partition coefficient of most compounds showed a strong pH dependence (Figure 2). For organic compounds with anion-like behavior, this pH relationship is negative, while for cation-like compounds such as dodecylamine, the relationship is positive, as confirmed by correlation coefficients (Table S2). Some compounds also exhibited a threshold relationship with decreasing sorption at very low and high pH values, and the highest partition coefficients in mildly acidic conditions. The highest partition coefficients across the measured pH range were found for the most complex organic compounds in our database, extracellular polymeric substances (Figure S1). In addition, there is a tendency of lower sorption for organic compounds with lower molecular weights, with some exceptions (e.g., in ferrihydrite and quartz experiments).

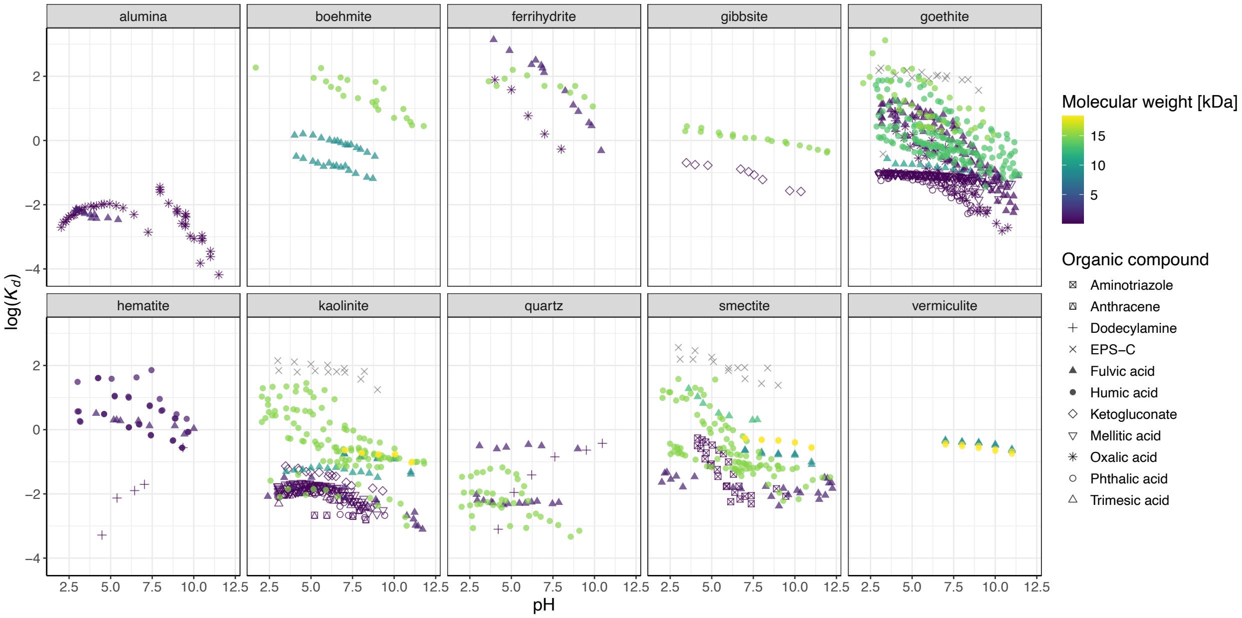

Figure 2: The partition coefficient log(K_d) of our organic-compound-specific sorption database as a function of pH for multiple common soil minerals and organic compounds (molecular weight indicated in color). The molecular weight of extracellular polymeric substances (EPS-C) was not measured in the collected studies and is therefore depicted in grey.

Our database includes sorption data of oxalic acid (depicted as an asterisk in Figure 2), an important root exudate, on three minerals—alumina, ferrihydrite, and goethite—that have decreasing solubility in this order. In comparison to the other organic compounds (including fulvic acid), oxalic acid had lower log(K_d) values for the two iron oxide minerals (ferrihydrite and goethite). However, in the case of alumina, sorption of oxalic acid appears to be greater than or equal to the sorption of fulvic acid and may reflect the patterns in solubility and aqueous complexation of oxalate with trivalent cations (Fe^{3+} and Al^{3+}) (Figure S2).

Exploratory Data Analysis and Predictive Modeling for Soil Organic Compounds

To improve our understanding of covariation among the numerical predictor variables—mineral surface area, initial concentration of organic compound, pH, ionic strength, and molecular weight—and log(K_d), we focused on organic compounds naturally occurring in soils to conduct a principal component analysis (PCA). To identify the drivers of mineral-associated carbon formation, we further estimated each predictor's importance based on a random forest regression.

The PCA, including all numerical predictors, explained ~45% of the variance in our data (filtered for soil organic compounds as defined in Table S1; n = 989) with the first two principal components (Figure 3b). Principal component 1 (PC1) was associated with pKa (Table S3), as indicated by its loadings (0.62), while mineral surface area and molecular weight contributed equally to PC2 (0.61). Within the ordination space, the data are structured in two distinct dimensions: (i) the first reflects aqueous conditions, which are distributed by ionic strength and pH, likely depicting variation across individual observations within experiments; and (ii) the second dimension reflects solid phase distribution by mineral surface area, showing variability across experiments.

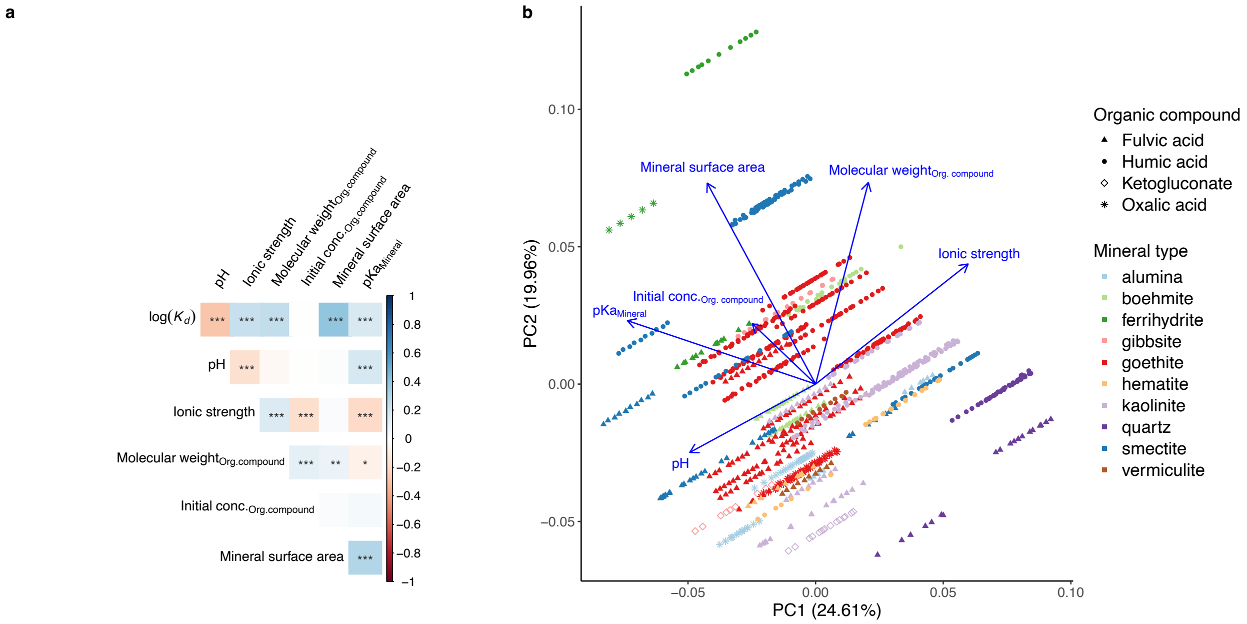

Figure 3: Exploratory data analysis for organic-compound-specific sorption database filtered for soil organic compounds (n = 989). a) Correlation matrix of independent, numeric variables and the dependent variable log(K_d). The coloring reflects the direction and strength of correlation, as indicated by the color bar which displays corresponding correlation coefficients. b) Principal component analysis biplot. Arrows represent the loadings; their length and direction indicate how much a variable contributes to a principal component. The percentage in parentheses of the principal components denotes the variance in the data that is explained by the respective principal component.

Focusing on soil organic carbon compounds (n = 989) and using each collected predictor individually, our random forest model predicted log(K_d) with a model performance (leave-one-experiment-out cross validation) of $R^2 = 0.77$ and an $RMSE$ of 0.59 (Figure 4a). Although our database includes a large range of minerals and organic compounds, most data points were near the 1:1 line. For minerals with greater data availability (e.g., goethite), we found these closest to the 1:1 line, indicating more accurate prediction. Minerals with lower surface area appeared at the bottom left, and more reactive minerals were located at the top right, showing higher sorption.

Mineral type and surface area were identified as the most important variables in predicting log(K_d) (Figure 4b), followed by features representing solution chemistry (pH and ionic strength), each of which explained a similar amount in the model. The organic compound characteristics and the pKa of minerals had the lowest explanatory power, with a relative importance of < 10%. We further tested our model for a narrowed pH range (between pH 3-8) to represent natural soil conditions more accurately (Figure 4c). The model results remained similar ($R^2 = 0.72$, $RMSE = 0.63$), however, the distribution of variable importance changed considerably (Figure 4d). The pH was least influential, while the mineral characteristics—mineral type, surface area, and pKa—dominated the prediction of log(K_d).

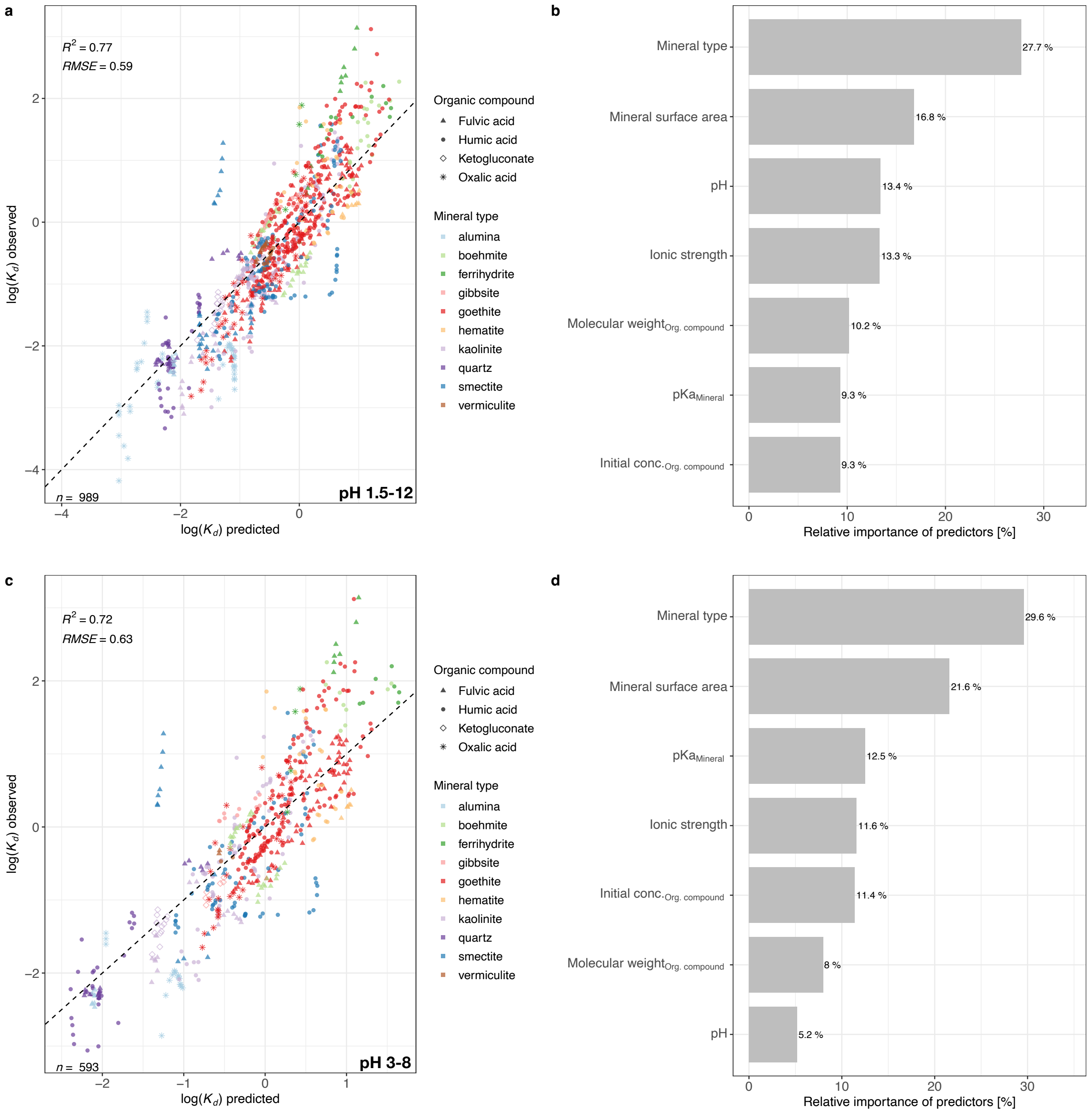

Figure 4: a) Random forest (RF) model for the entire measured pH range (pH 1.5-12) to predict log(K_d) for sorption of a variety of soil organic carbon compounds on a range of soil minerals. Dashed line represents 1:1 line. b) Relative variable importance of predictors for RF model pH 1.5-12. c) RF model for narrowed pH range reflecting common soil conditions (pH 3-8). Dashed line represents 1:1 line. d) Relative variable importance of predictors for RF model pH 3-8.

Greatest Sorption on Iron Oxides Across Organic-Compound-Specific Sorption Database

Our organic-compound-specific sorption database includes 1,673 data points that span a range of experimental conditions, minerals, and organic compounds, enabling us to improve our predictive understanding of mineral associations and their drivers. This first-of-its-kind database covers both simple and more complex organic compounds, with the latter showing greater sorption (Figure S1). Across the entire dataset, with sorption data on ten different mineral types, organic compounds showed the greatest sorption on Fe oxides (Figure 1b). This observation is consistent with the classification and properties of minerals in Kleber et al. (2021), namely that Fe oxides have large surface areas and high reactivity. Iron oxides have been shown to exhibit a high abundance of reactive sites, and soils rich in such minerals contain a greater amount of MAOC (Keiluweit et al. 2012; Kirsten et al. 2021; Jia et al. 2024). On the other hand, smectite and vermiculite (expandable clay minerals with generally high sorption capacity due to large surface areas; Wiesmeier et al. 2019), revealed lower sorption than expected. However, this finding is likely because the samples with smectite and vermiculite in our database had unusually low surface areas (Table 1). Further, mineral surface area is challenging to measure in soil (Kirschbaum et al. 2020), and the reactive surface area measured in soil can differ substantially from the pure mineral's specific surface area due to hydration and blockage of adsorption sites by organic matter in soil samples (Heister 2014; Mendez et al. 2020).

Consistent Partition Coefficient-pH Relationship

The partition coefficient of the majority of organic compounds showed a negative relationship with pH (Figure 2). This relationship can mostly be explained by electrostatic interactions, because many soil organic compounds have an overall negative charge, given that most are acids with negative ions. At low pH, the positively charged mineral surface will electrostatically attract the negatively charged surface of the organic compound, while minerals with variably charged surfaces will become negatively charged at higher pH, leading to electrostatic repulsion (Christl and Kretzschmar 2001; Chen et al. 2017). For a few organic compounds, we observed a threshold relationship such that after a certain pH is reached, K_d decreases as pH decreases, which may be related to mineral dissolution at low pH. This observation was confirmed in individual studies, where the simultaneous release of cations was measured, indicating mineral dissolution (Schulthess and Huang 1991). This finding is also consistent with Abramoff et al.'s (2021) synthesis study which reported a threshold effect of pH, where sorption decreased at very acidic pH ($pH < 4$).

Mineral Dissolution as a Potential Control of MAOC Release

To further examine this low pH sorption behavior, we analyzed the partition coefficient of oxalic acid (Figure 2). Our analysis of this common root exudate indicated that MAOC disruption can be caused by mineral dissolution rather than desorption. The presence of oxalic acid can enhance the solubility of some minerals, which may promote disruption of mineral associations with decreasing pH. For example, in the case of ferrihydrite, oxalic acid forms complexes with the released iron, contributing to further mineral dissolution (Figure S2a) and hence the release of previously bound carbon (Strawn et al. 2019). Similarly for alumina, we expect the increased solubility resulting from aqueous complexation between oxalic acid and aluminum to promote greater mineral dissolution and thus greater MAOC disruption and release for this mineral. This expectation was supported by our geochemical simulations using thermodynamic constants, which revealed complete dissolution of alumina at ~pH 4.5, aligning with the threshold in the collected experiments where K_d decreases (Figure S2b). In such controlled systems, mineral dissolution might be the main driver of MAOC release rather than desorption, but this connection requires further validation. For example, with all else constant, an experiment could compare the amount of oxalic acid adsorbed to the mineral surface with that associated with released ions in the aqueous phase as a function of each mineral's solubility. Apart from mineral dissolution effects, the threshold effect of pH may also result because of protonation of the organic compound at low pH, leading to less attraction to positively charged mineral surfaces.

Mineral Characteristics as Most Influential Drivers of Sorption

Our random forest models demonstrated that log(K_d) is predictable under controlled laboratory settings using parameters associated with mineral properties, aqueous conditions, and organic-compound characteristics ($R^2 > 0.7$; Figure 4). The high importance of mineral type and surface area identified in our models is supported by qualitative understanding of MAOC formation (Wiesmeier et al. 2019; Kleber et al. 2021). The fundamental role of minerals is further corroborated by other data-driven modeling studies that found that soil order—a soil classification that incorporates information on soil weathering and parent material—was among the most important parameters, along with organic carbon concentration and pH (Abramoff et al. 2021). Furthermore, not only in the context of MAOC formation but also for MAOC stability, mineral type has been found to represent the most influential factor in natural soils (Bramble et al. 2025).

Our model spanning the full measured pH range (pH 1.5-12) indicated that pKa—a more mineral-specific property dependent on surface chemistry characteristics—was not influential in predicting sorption. This finding could potentially be explained by pKa variability for the same mineral type, depending on edge sites and the specific configuration of the mineral. For example, montmorillonite that has a Mg substitution, and thus different edge sites, can have pKa values up to 13.2, whereas when not substituted, pKa for these edge sites is only 7 (Liu et al. 2013). In our dataset, we used averages of pK1 values across different edge sites, which potentially did not reflect each mineral's protonation of edge sites accurately enough. However, when we tested our model only with data across the pH range of 3-8 to represent conditions found in natural soils, pKa had a higher importance, which led to the mineral phase controlling the sorption prediction (Figure 4d).

We found that K_d was less associated with aqueous properties under expected environmental conditions. In the random forest model, across the full pH range measured in the experiments, pH was among the most important variables (Figure 4b). After narrowing the pH range to represent pH values in natural soils, pH lost its explanatory power almost entirely, with a relative importance of only 5.3% (Figure 4d). This finding was expected due to the strong negative pH-log(K_d) relationship governed by the extreme values at both ends of the pH range, which were much weaker after narrowing to pH 3-8 (Figure S3). The second aqueous property, ionic strength, contributed similarly to the model outcome in both cases. Its intermediate influence on K_d is in accordance with findings reported in individual sorption studies, where some studies found that higher ionic strength corresponded with slightly greater K_d values due to greater electrostatic potential (Feng et al. 2005; Nordén et al. 1994), while others found that sorption was independent of ionic strength (Filius et al. 2000).

We found that molecular weight played a minor role in our model, despite it being a key parameter in characterizing organic compounds. Some individual studies have pointed to higher sorption of higher-molecular weight compounds, but the influence of molecular weight might be more related to the chance that a heavier compound might also have a greater variety of functional groups (Zhang et al. 2012; Chen et al. 2017). However, it is also possible for low-molecular weight compounds to have a variety of functional groups and thus exhibit higher log(K_d) values (Kleber et al. 2021). Further, there is uncertainty with the determination of molecular weights for humic and fulvic acids (Perminova et al. 2003), and the collected molecular weights might not have captured the specific compound's weight accurately enough. Additionally, molecular weight might have not been important in our model because there is more variability in mineral properties than in the molecular weights of organic compounds within our database.

Limitations

We acknowledge that our study has several important limitations. First, the range of more complex organic compounds in our dataset is limited, as well as the number of parameters characterizing the organic compounds. As a result, our model included more predictor variables describing the mineral phase than the organic phase, which could have led to model biases toward mineral parameters. Similarly, we acknowledge that the data is not evenly distributed among organic compounds and mineral types, which might have given more weight to overrepresented organic compounds and minerals. Second, our study is based on controlled laboratory experiments, while environmental conditions in the field are much more complex. For example, parameters such as ionic strength have a limited range under experimental conditions, which may not be representative of the variability in ionic strength found in natural soils. Further, even though mineral availability and surface area influence how much MAOC theoretically can form, environmental conditions and microbiota determine the amount that can ultimately be sorbed and that will stay sorbed (Schmidt et al. 2011; Lehmann et al. 2020; Ding et al. 2021). Third, a large proportion of the collected experiments used humic and fulvic acid, which are both operationally defined, making the extrapolation from these controlled systems to natural soils more challenging (Sutton and Sposito 2005; Kelleher and Simpson 2006; Lehmann and Kleber 2015). While we recognize the limitation in using HA and FA, the wealth of sorption experiments with HA and FA has great potential to improve our understanding of MAOC controls. However, our model presents a quantitative understanding, albeit derived from laboratory settings, for advancing our current understanding of organo-mineral associations (Kleber et al. 2021). Insights from our model results can also provide guidance in practical applications when selecting locations for more stable SOC accrual, based on recently published global maps of the dominant secondary mineral type in a soil profile (Liao et al. 2024). More importantly, our analysis lays the groundwork for a community sorption database strategy that can help inform MAOC models by testing the suitability of parameters available at the global scale, improve the prediction of MAOC extent and persistence, and, in turn, the effectiveness of using SOC accrual as a CDR strategy.

Implications

To effectively encourage MAOC accrual as a long-term carbon dioxide removal strategy, it is essential to understand its key drivers. Laboratory experiments—with limited complexity and controlled conditions—can play a critical role in untangling nature's complexity and informing our understanding of which parameters are most important to consider when modeling MAOC accrual for global-scale projects. Our compiled datasets allowed us to conduct a comprehensive analysis, which revealed a stronger influence of the mineral phase on sorption than the characteristics of organic compounds. Our results are generally consistent with other studies that used natural soils (Abramoff et al. 2021; Bramble et al. 2025) but indicate that including additional mineral-specific properties such as mineral surface area could further improve our predictive ability of MAOC formation. Overall, our study suggests the significant role of mineral properties in predicting sorption magnitude. This finding proposes the importance of characterizing soil properties such as mineral type and surface area when CDR is planned. These properties are quasi-static and mappable across the globe, unlike the rapidly cycling organic phase (Sulman et al. 2014; Zhou et al. 2024). As soil mapping has improved dramatically over the last decade, using these mineral-specific soil characteristics available at the global scale could inform MAOC formation models, or more broadly soil biogeochemical models, to effectively increase MAOC as a CDR strategy and to improve climate projections (Chaney et al. 2016; Ito and Wagai 2017; Liao et al. 2024).

Supporting Information

Additional information on the organic compound characteristics, the Pearson's correlation coefficients of the partition coefficient with pH, the principal component analysis, the effect of oxalic acid on mineral dissolution, the correlation analysis for pH 3-8, and a list of the collected papers in the database (PDF)

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Supporting Information for:

Mineral properties identified as most influential drivers of mineral-associated organic carbon formation using a community-based sorption database

Authors: Maria E. Macfarlane[1], Haruko M. Wainwright[1,2], Jon K. Golla[3], Katerina Georgiou[4], César Terrer[1], Jennifer Pett-Ridge[5,6,7], Mavrik Zavarin[3]

Affiliations

[1]Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA

[2]Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA

[3]Seaborg Institute, Lawrence Livermore National Laboratory, Livermore, CA, USA

[4]Physical Department, Oregon State University, Portland, OR, USA

[5]Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, CA, USA

[6]Life and Environmental Sciences Department, University of California Merced, Merced, CA, USA

[7]Innovative Genomics Institute, University of California, Berkeley, CA USA

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- Tables S1 to S3
- Figures S1 to S3
- List of references included in the database
- References for the supporting information

Table S1: List of organic compounds and their molecular weights (including references). Column "Soil" indicates whether a compound naturally occurs in soil (Y=Yes, N=No). Column "Charge" identifies whether a compound acts as an anion or cation at neutral pH. EPS-C = Carbon in extracellular polymeric substances; given that there was no molecular weight available due to the high complexity of EPS, we excluded EPS-C from the exploratory data analysis and Random Forest regression, even though it is a compound that naturally occurs in soil.

Organic compound	**Soil**	**Charge**	**Molecular weight [kDa]**
Humic acid	Y	anionic	1.1 (Averett et al. 1994), 13.2 (Weng et al. 2006), 15.0 (Tarasevich et al. 2016), 18.3 (Zhang et al. 2012)
Fulvic acid	Y	anionic	0.683 (Weng et al. 2006), 1.58 (Perminova et al. 2003), 9.01 (Zhang et al. 2012), 10.2 (Chen et al. 2023)
Mellitic acid	N	anionic	0.34 (Sigma Aldrich)
Phthalic acid	N	anionic	0.17 (Sigma Aldrich)
Oxalic acid	Y	anionic	0.09 (Sigma Aldrich)
Anthracene	N	anionic	0.18 (Sigma Aldrich)
EPS-C	Y	anionic	NA
Aminotriazole	N	anionic	0.08 (Sigma Aldrich)
Ketogluconate	Y	anionic	0.18 (Sigma Aldrich)
Trimesic acid	N	anionic	0.21 (Sigma Aldrich)
Dodecylamine	N	cationic	0.19 (Sigma Aldrich)

Table S2: Pearson's correlation coefficients *r* of log(K_d) with pH of each mineral-sorbate pair. *n*=number of measurements for specific mineral-sorbate pair.

Mineral	**Sorbate**	***n***	***r***	***p*-value**	**significance level**
alumina	Fulvic acid	10	-0.88	<0.001	***
alumina	Oxalic acid	47	-0.5	<0.001	***
quartz	Dodecylamine	6	0.92	0.01	**
quartz	Fulvic acid	19	0.12	0.63	ns
quartz	Humic acid	39	-0.48	0	**
kaolinite	Anthracene	5	-0.13	0.84	ns
kaolinite	EPS-C	14	-0.71	0	**
kaolinite	Fulvic acid	39	-0.36	0.03	*
kaolinite	Humic acid	119	-0.59	<0.001	***
kaolinite	Ketogluconate	15	-0.97	<0.001	***
kaolinite	Mellitic acid	114	-0.69	<0.001	***
kaolinite	Phthalic acid	48	-0.77	<0.001	***
kaolinite	Trimesic acid	14	-0.67	0.01	**
goethite	EPS-C	18	-0.22	0.39	ns
goethite	Fulvic acid	119	-0.83	<0.001	***
goethite	Humic acid	212	-0.64	<0.001	***
goethite	Mellitic acid	155	-0.68	<0.001	***
goethite	Oxalic acid	49	-0.93	<0.001	***

goethite	Phthalic acid	64	-0.81	<0.001	***
goethite	Trimesic acid	13	-0.96	<0.001	***
smectite	Aminotriazole	27	-0.8	<0.001	***
smectite	EPS-C	14	-0.87	<0.001	***
smectite	Fulvic acid	41	-0.36	0.02	*
smectite	Humic acid	106	-0.61	<0.001	***
vermiculite	Fulvic acid	10	-0.92	<0.001	***
vermiculite	Humic acid	10	-0.94	<0.001	***
gibbsite	Humic acid	19	-0.98	<0.001	***
gibbsite	Ketogluconate	9	-0.95	<0.001	***
boehmite	Fulvic acid	29	-0.37	0.05	*
boehmite	Humic acid	22	-0.88	<0.001	***
hematite	Dodecylamine	5	0.97	0.01	**
hematite	Fulvic acid	9	-0.92	<0.001	***
hematite	Humic acid	37	-0.47	0	**
ferrihydrite	Fulvic acid	13	-0.97	<0.001	***
ferrihydrite	Humic acid	11	-0.75	0.01	**
ferrihydrite	Oxalic acid	5	-0.99	<0.001	***

Table S3: Loadings for each predictor variable and principal component.

Predictor variable / Principal component	**PC1**	**PC2**	**PC3**	**PC4**	**PC5**	**PC6**
pH	-0.41	-0.21	0.06	-0.81	-0.31	-0.15
Ionic strength	0.50	0.37	0.35	-0.15	-0.61	0.31
Molecular weight	0.17	0.61	-0.33	-0.48	0.49	0.12
Initial conc.$_{\text{Org. compound}}$	-0.21	0.18	-0.78	0.18	-0.52	0.07
Mineral surface area	-0.36	0.61	0.30	0.20	-0.10	-0.60
pKa$_{\text{Mineral}}$	-0.62	0.19	0.24	0.12	0.08	0.71

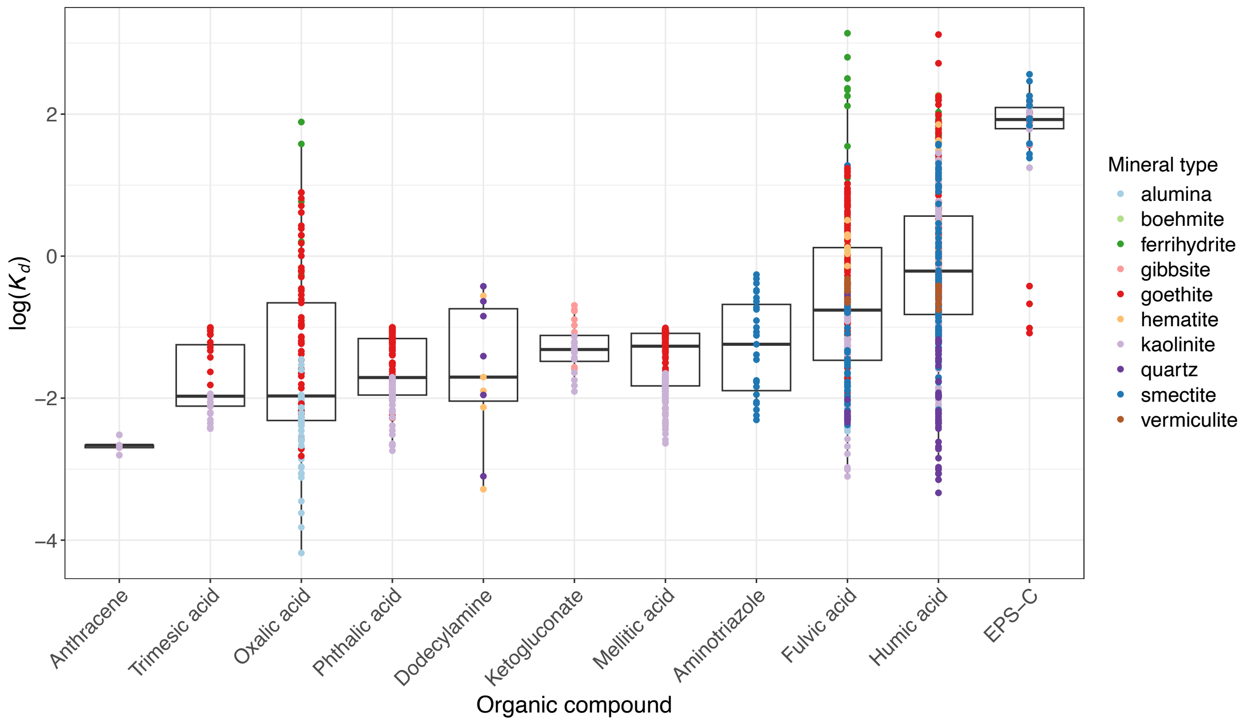

Figure S1: Variation and magnitude of log(K_d) across organic compounds. EPS-C = Carbon within extracellular polymeric substances.

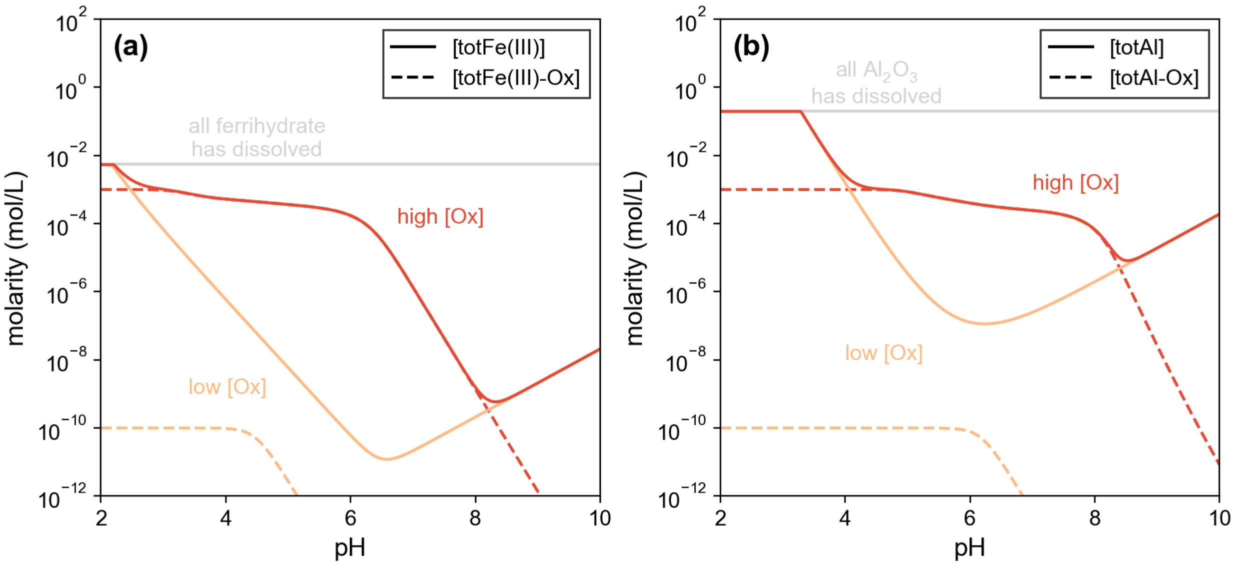

Figure S2: Theoretical modeling of the effect of variable oxalic acid ('Ox') concentrations on the solubility of ferrihydrite (a) and alumina (b). These computations are based on a 0-D Reaktoro geochemical model in which the amount of oxalic acid is varied from low ([Ox] = 1E-10 M) to high ([Ox] = 1E-3 M; this value corresponds to the initial sorbate concentration used in the experiments of Jones & Brassington 1998 and Alliot et al. 2005) quantities. Fixed amounts of 5.88E-1 g/L ferrihydrite and 10 g/L alumina are prescribed and directly correspond to solid-solution ratios in the experiments of Jones & Brassington 1998 and Alliot et al. 2005, respectively.

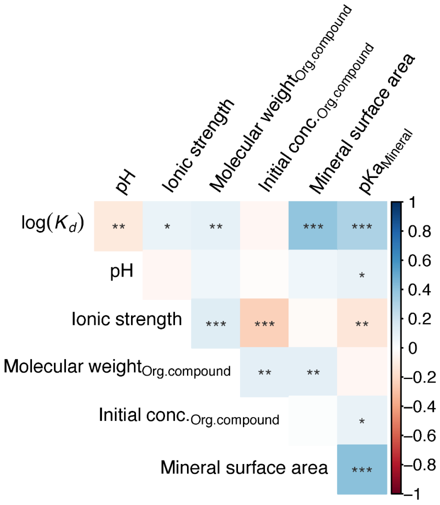

Figure S3: Correlation analysis with data for pH 3-8 (*n* = 593).

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