Amino acids in iron oxide mineralization: (incomplete) crystal phase selection is achieved even with single amino acids

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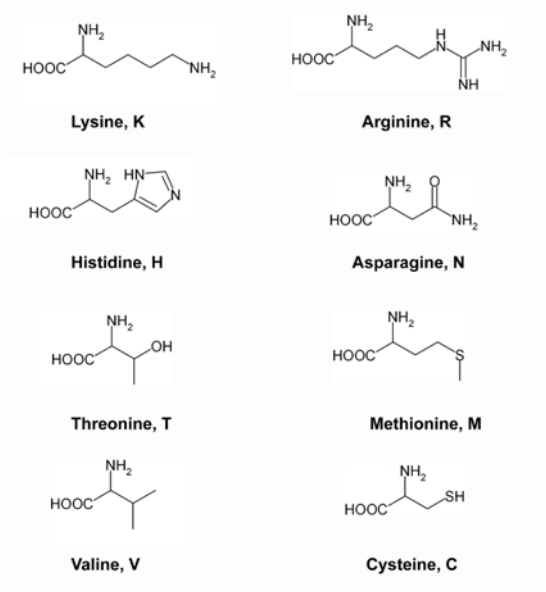
Supporting Information



Scheme S1. Amino acids used in this study. All amino acids used were L-amino acids.

Table S1: X ray fluorescence assay of sulfur and iron (expressed as their oxide).

	L-cysteine	L-methionine
0 mM	98.68 % Fe2O3 - 0.08 % SO3	
0.1 mM	96.5 % Fe2O3 : 2.037 % SO3	97.68 % Fe2O3 : 0.57 % SO3
1 mM	96.43 % Fe2O3 : 1.93 % SO3	98.47 % Fe2O3 : 0.37 % SO3
10 mM	98 % Fe2O3 : 1 % SO3	97.35 % Fe2O3 : 1.15 % SO3
100 mM	6.8 % Fe2O3 : 89.64 % SO3	94.76 % Fe2O3 : 3.91 % SO3

Table S2. Sizes (error) and strain (anisotropy) analysis of the samples determined from Rietveld refinement. Mag: magnetite, Goe: goethite, Lep: lepidocrocite, Fer: ferrihydrite, n/a: not applicable due to too low peak intensity or too broad reflections.

AA	**Crystallite sizes (Å)**			**Apparent strain (%%)**		
	1 mM	10 mM	100 mM*	1 mM	10 mM	100 mM*
Control sample	Mag: 566.06 (0.36) Goe: 64.47 (0.15)			Mag: 36.0825 (0.0028) Goe: 80.7454 (0.1)		
L-val	Mag: 209.27 (0.15)	Mag: 123.89 (0.08)	Mag: 27.07 (0.02) Goe: n/a Lep: 84.48 (0.06)	Mag: 12.0749 (0.0018)	Mag: 12.4325 (0.0168)	Mag: 21.5293 (0.0137) Goe: n/a Lep: 21.5300 (.0423)
L-lys	Mag:172.56 (0.11)	Mag: 148.49 (0.3) Goe: 148.39 (0.3)	*Mag: 27.07 (0.02)* Goe: n/a Lep: 84.48 (0.12)	Mag: 53.1941 (0.0360)	Mag: 138.2929 (0.1614) Goe: 138.2929 (0.0694)	*Mag: 21.5293 (0.0131)* *Goe: n/a* Lep:21.5300 (0.0414)
L-met	Mag: 291	Mag: 62 Goe: 62.24	*Mag: 30* Lep: 44.59	Mag: 12.42	Mag: 24.25 Goe: 24.25	*Mag: 40.50* Lep: 40.50
L-asp	Mag: 175.13 (0.13) Goe: 24.73 (0.04)	Mag: 62.97 (0.08)	Mag: 55.42 (0.06) Goe: 46.61 (0.10)	Mag: 175.13 (0.13) Goe: 48.2004 (0.0881)	Mag: 21.5293 (0.0050)	*Mag: 21.5293 (0.0220)*

			Lep: 69.10 (0.10)			Goe: 21.530 (0.0114) Lep: 68.0787 (0.0674)
L-arg	Mag: 255.24 (.04)	Mag: 65.46 (0.06) Goe: 126.66 (0.34)	*Mag: 53.01 (0.05)* Goe:35.66 (0.06) Lep: 69.08 (0.07)	Mag: 12.2453 (0.0101)	Mag: 35.4443 (0.0179) Goe: 149.0564 (0.1372)	*Mag: 1038,9541 (1.3328)* Goe: 70.2676 (0.1419) Lep:21.5298 (0.0281)
L-his	Mag: 294.24 (0.02)	Mag: 104.50 (0.09)	Fer: n/a	Mag: 52.9516 (0.0476)	Mag: 29.0648 (0.373)	Fer: n/a
L-thr	Mag: 95.13 (0.13) Goe: 13.95 (0.01)	Mag: 44.04 (0.2) Goe:47.08 (0.03) Lep: 80.27 (0.13)	Fer: n/a	Mag: 48.2074 (0.0572) Goe: 48.2029 (0.0938)	Mag: 21.5293 (0.0137) Goe: 21.5301 (0.0560) Lep: 21.4295 (0.0319)	Fer: n/a
L-cys	Mag: 231.69 (0.17) Goe: 113.37 (0.16) Lep: 305.44 (0.31)	Lep: 52.11 (0.06)		Mag: 13.6854 (0.0051) Goe: 72.5522 (0.0836) Lep: 72.5522 (0.0446)	.Lep: 14.0265 (0.0174)	

* Maximum concentrations are 80 mM for L-threonine and 60 mM for L-histidine.