The origin of heredity in protocells
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SI Table 1

| Initial Values | Symbol | Name | Value | Notes |
|----------------|--------|------|-------|-------|
| $V_{\text{crys}}^{\text{cyto}}(1)$ | Initial mean crystal volume | 1x10^{-15} \text{ cm}^3 | Cuboid nanocrystal of length ~500nm |
| $[\text{crys}]^{\text{mem}}(1)$ | Initial concentration of crystal in membrane | 1x10^{-9} \text{ mol dm}^{-3} | Set very low |
| $[\text{aa}]^{\text{cyto}}(1)$ | Initial concentration of amino acid in the cytosol | 1x10^{-6} \text{ mol dm}^{-3} | Set low |
| $[\text{fa}]^{\text{cyto}}(1)$ | Initial concentration of fatty acid in the membrane | 1x10^{-6} \text{ mol dm}^{-3} | Set low |
| $S_{\text{A}}^{\text{cyto}}(1)$ | Initial cytoplasm surface area | 4.84x10^{-6} \text{ cm}^2 |
| $[\text{crys}]^{\text{cyto}}(1)$ | Initial concentration of crystal in cytosol | 1x10^{-6} \text{ mol dm}^{-3} | Typical particulate FeS found in hydrothermal vent samples [1] |
| $V_{\text{crys}}^{\text{cyto}}(eq)$ | Total crystal population volume (fixed) | 6x10^{-10} \text{ cm}^3 |

| Transport | Symbol | Name | Value | Notes |
|-----------|--------|------|-------|-------|
| $P_{\text{aa}}^{\text{cyto}}$ | Permeability coefficient for amino acids from cytosol | 1x10^{-9} \text{ cm s}^{-1} | Set very low |
| $P_{\text{fa}}^{\text{cyto}}$ | Permeability coefficient for fatty acids from cytosol | 1x10^{-9} \text{ cm s}^{-1} | Set very low |
| $P_{\text{crys}}^{\text{cyto}}$ | Association constant for crystal permeation from cytosol | 1x10^{-12} \text{ cm s}^{-1} | Set very low |
| $P_{\text{mem}}^{\text{crys}}$ | Association constant for crystal permeation from membrane | 1x10^{-12} \text{ cm s}^{-1} | Set very low |
| $P_{\text{surf}}^{\text{crys}}$ | Permeability coefficient for FeS diffusion to crystal surface | 1x10^{-12} \text{ cm s}^{-1} |
### Crystal Growth

| Symbol | Name | Value | Notes |
|--------|------|-------|-------|
| $k^\text{Grow}$ | Rate constant for crystal growth | $1 \times 10^{-6} \text{ s}^{-1}$ | |
| $D_{\text{min}}^{\text{crys}}$ | Minimum crystal size | $1 \times 10^{-16} \text{ cm}^3$ | Minimum nanocrystal length ~50nm |
| $K_{\text{crys}}$ | Saturation constant of FeS crystal nucleation | $1 \times 10^{-8} \text{ mol dm}^{-3}$ | |

### Catalysis and Amino Acid Interactions

| Symbol | Name | Value | Notes |
|--------|------|-------|-------|
| $[CO_2]_{\text{in}}$ | Concentration of aqueous CO$_2$ in cytosol | $1 \times 10^{-3} \text{ mol dm}^{-3}$ | 10x CO$_2$ concentration at Lost City hydrothermal field [2] |
| $K_{CO_2}$ | CO$_2$ binding constant for iron-sulphur catalyst | $3 \times 10^{-4} \text{ mol dm}^{-3}$ | ~0.3mM affinity of CO$_2$ for ferredoxins [3] |
| $K_{aa}$ | Binding constant of amino acids for crystals | $1 \times 10^{-4.5} \text{ to } 10^{-2} \text{ mol dm}^{-3}$ | (varied in simulations) |
| $\lambda_{aa}$ | Fraction of organic yield that is amino acid | 1/10 | |
| $\lambda_{fa}$ | Fraction of organic yield that is fatty acid | 1/4 | |
| $R_{\text{cat}}$ | Organic turnover rate per unit area | $1 \times 10^{11.8} \text{ to } 10^{9.3} \text{ mol cm}^{-2} \text{ s}^{-1}$ | (varied in simulations) |

### Cell Geometry

| Symbol | Name | Value | Notes |
|--------|------|-------|-------|
| $r_{\text{mem}}$ | Thickness of fatty acid bilayer | $1 \times 10^{-6} \text{ cm}$ | ~10nm thick bilayer in yeast [4] |
| $\phi_{fa}$ | Headgroup area of fatty acid | $2 \times 10^{-15} \text{ cm}^2$ | ~0.2nm$^2$ surface area of arachidic acid [5] |
| $V_{\text{cyto}}$ | Volume of protocell cytosol | $1 \times 10^{-9} \text{ cm}^3$ | Cell of ~6000 μm$^3$ |

### Concentrations

| Symbol | Name | Value | Notes |
|--------|------|-------|-------|
| $[aa]_{\text{sink}}$ | Concentration of amino acids in sink | $1 \times 10^{-6} \text{ mol dm}^{-3}$ | ~1μM concentrations in hydrothermal fluids and plume at Lost City [6] |
| $[fa]_{\text{sink}}$ | Concentration of fatty acids in sink | $1 \times 10^{-6} \text{ mol dm}^{-3}$ | |

### Constants

| Symbol | Name | Value | Notes |
|--------|------|-------|-------|
| $A_N$ | Avogadro’s number | $6.023 \times 10^{23} \text{ mol}^{-1}$ | |
References for SI Table 1

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