Article

Bio-Precipitation of Carbonate and Phosphate Minerals Induced by the Bacterium Citrobacter freundii ZW123 in an Anaerobic Environment

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Table S1 Parameter settings of molecular dynamic simulation for adsorption of Glu onto various struvite surfaces.

<table>
<thead>
<tr>
<th>Ensemble</th>
<th>Temperature</th>
<th>Time Step</th>
<th>Dynamics Time</th>
<th>Thermostat</th>
</tr>
</thead>
<tbody>
<tr>
<td>NVT</td>
<td>298 K</td>
<td>1 fs</td>
<td>50 ps</td>
<td>Andersen</td>
</tr>
</tbody>
</table>

Table S2 Physiological and biochemical identification of ZW123 and Citrobacter freundii species

<table>
<thead>
<tr>
<th>Tests</th>
<th>ZW123</th>
<th>Citrobacter freundii*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gram</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>V-P</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>H2S production</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>Amylase</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Indole</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Lysine decarboxylase</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Ornithine decarboxylase</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Bacterial motility</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>NH3 release test</td>
<td>+</td>
<td>+</td>
</tr>
</tbody>
</table>

Note: * Published paper of Brenner et al [57].

Figure S1. Phylogenetic tree of Citrobacter freundii ZW123 based on the sequence alignment.
Figure S2. SEM image of *Citrobacter freundii* ZW123 bacteria (a) and Gram staining test (b) and NH₃ test (c) before adding the Nessler’s reagent; d: after adding the Nessler’s reagent. 1, control group; 2 and 3, experimental groups).

Figure S3. Rietveld refinement of XRD data at Mg/Ca molar ratio 0 (a), 3 (b), 6 (c), 9 (d) and 12 (e).
Figure S4. Molecular dynamics simulation of adsorption of Glu onto crystal: a: temperature fluctuation of the adsorption of Glu onto (111) faces; b: energy fluctuation of the adsorption of Glu onto (111) faces.