Electronic Supplementary Information

Enantioselective incorporation of dicarboxylate guests by octacalcium phosphate

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1. Magnified FTIR spectra

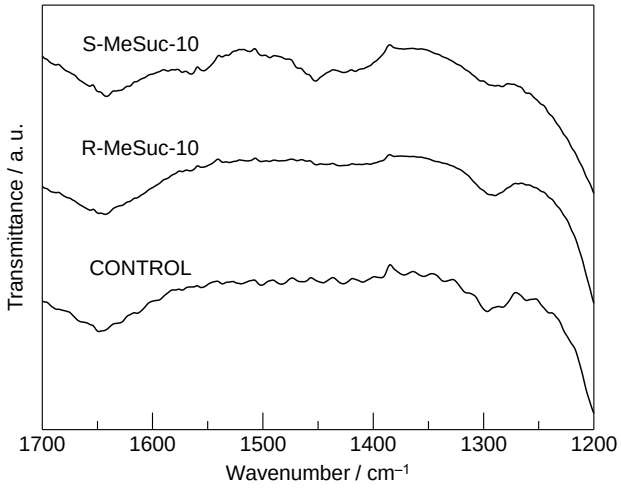

Figure S1 Magnified FTIR spectra of CONTROL, R-MeSuc-10, and S-MeSuc-10 in the range of 1200–1700 cm^{-1}.

2. TG curves

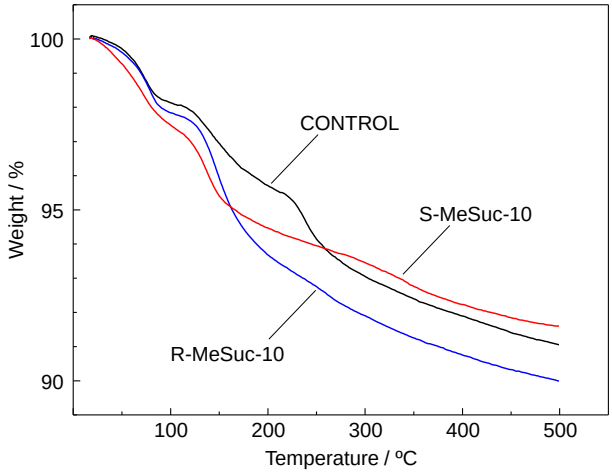

Figure S2 TG curves of CONTROL, R-MeSuc-10, and S-MeSuc-10 on heating from room temperature to 500 °C.

3. Calculation method for the number of crystalline water molecules

We calculated the number of crystalline water molecules in OCP according to a previously reported method.[1] The amount of crystalline water can be estimated from the TG analysis, as the weight loss up to 400 °C corresponds to thermal dehydration of crystalline water as well as the loss of water generated from the condensation reaction of hydrogen phosphate ions, according to the following reaction:

$$2HPO_4^{2-} \rightarrow P_2O_7^{4-} + H_2O\uparrow$$

It is supposed that the weight loss up to 400 °C owing to thermal decomposition of dicarboxylate ions incorporated into OCP is negligible small. The fraction of crystalline water was empirically estimated based on a detailed thermal analysis combined with the XRD and FTIR results. The weight of crystalline water was assumed to be 85% of the weight loss observed between room temperature and 400 °C. This calculation method is convenient for semiquantitative determination of the amount of crystalline water.

The weight losses observed for CONTROL, R-MeSuc-10, and S-MeSuc-10 from room temperature to 400 °C are 8.1, 9.3, and 7.8 mass%, respectively. The compositional formula of CONTROL and R-MeSuc-10 is regarded as $Ca_8(HPO_4)_2(PO_4)_4 \cdot mH_2O$. In

contrast, as the Ca/P ratio of S-MeSuc-10 is 1.42, the compositional formula of this sample is assumed to be $Ca_8(HPO_4)_{1.63}(DCI)_{0.37}(PO_4)_4 \cdot mH_2O$, where DCI is (S)-(–)-MeSuc. The formula weights of the samples are as follows:

CONTROL, R-MeSuc-10: 892.5 + 18.0*m* (g/mol)
S-MeSuc-10: 905.1 + 18.0*m* (g/mol)

As the weight of crystalline water was assumed to be 85% of the weight loss observed between room temperature and 400 °C, the *m* values in the compositional formulae are obtained by solving the following equations.

CONTROL: $18.0m/(892.5 + 18.0m) \times 100 = 8.1 \times 0.85$
R-MeSuc-10: $18.0m/(892.5 + 18.0m) \times 100 = 9.3 \times 0.85$
S-MeSuc-10: $18.0m/(905.1 + 18.0m) \times 100 = 7.8 \times 0.85$

Therefore, the *m* values of CONTROL, R-MeSuc-10, and S-MeSuc-10 were estimated as 3.7, 4.3, and 3.6, respectively.

4. NMR spectra

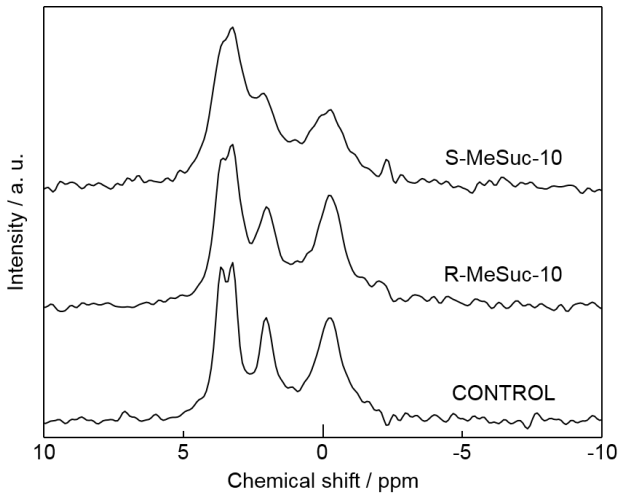

Figure S3 ^{31}P MAS NMR spectra of CONTROL, R-MeSuc-10, and S-MeSuc-10.

We collected the ^{31}P MAS NMR spectra of CONTROL, R-MeSuc-10, and S-

MeSuc-10. The peaks detected in these samples are derived from the OCP phase, as based on a previous report.[2]

References

1 H. Monma, *Gypsum Lime*, 1990, **229**, 396. [in Japanese]

2 T. W. T. Tsai, F.-C. Chou, Y.-H. Tseng and J. C. C. Chan, *Phys. Chem. Chem. Phys.*, 2010, **12**, 6692.