

Supplementary Table S2. Bond lengths and angles for the Ca₄O₄ cluster.

Bond	Length (Å)	Angle	Value (°)	Angle	Value (°)
Ca1-O1	2.157	O1-Ca1-O2	87.885	Ca1-O1-Ca2	92.069
Ca1-O2	2.156	O1-Ca1-O3	87.894	Ca1-O1-Ca3	92.061
Ca1-O3	2.158	O2-Ca1-O3	92.044	Ca2-O1-Ca3	92.127
Ca2-O1	2.157	O1-Ca2-O2	87.865	Ca1-O2-Ca2	92.108
Ca2-O2	2.156	O1-Ca2-O4	87.845	Ca1-O2-Ca4	92.002
Ca2-O4	2.159	O2-Ca2-O4	87.908	Ca2-O2-Ca4	92.023
Ca3-O1	2.158	O1-Ca3-O3	87.886	Ca1-O3-Ca3	92.080
Ca3-O3	2.157	O1-Ca3-O4	87.846	Ca1-O3-Ca4	92.044
Ca3-O4	2.158	O3-Ca3-O4	87.824	Ca3-O3-Ca4	92.108
Ca4-O2	2.160	O2-Ca4-O3	87.911	Ca2-O4-Ca3	92.013
Ca4-O3	2.157	O2-Ca4-O4	87.914	Ca2-O4-Ca4	92.076
Ca4-O4	2.155	O3-Ca4-O4	87.885	Ca3-O4-Ca4	92.108