

Supplementary Table S1. Atomic positions and isotropic thermal parameters for dolomite coming out from Rietveld refinement of XRPD data. As regards the accordance parameters for Rietveld data refinements, see Table 4.

	DS1	DS2	DS3	DP1
Atomic positions				
z_C	0.2439(5)	0.2435(5)	0.2436(3)	0.2406(6)
x_O	0.2409(7)	0.2371(7)	0.2515(8)	0.2517(8)
y_O	-0.0324(8)	-0.0386(8)	-0.0336(9)	-0.032(1)
z_O	0.2450(2)	0.2449(3)	0.2433(3)	0.2438(3)
Isotropic thermal parameters				
Uiso*100 (site Ca)	3.4(1)	3.2(1)	2.8(1)	2.8(1)
Uiso*100 (site Mg)	2.6(1)	3.6(2)	2.6(2)	2.6(2)
Uiso*100 (C)	0.1(1)	0.5(2)	0.3(2)	1.1(2)
Uiso*100 (O)	3.4(1)	3.3(1)	2.2(1)	2.7(1)

Supplementary Table S2. Oxygen atomic positions and anisotropic thermal parameters for dolomite coming out from SC-XRD data refinement. As regards the accordance parameters for data refinements, see Table 5.

	DS1	DS2	DS3	DP1
Oxygen atomic positions				
x_O	0.2489(5)	0.2824(5)	0.2833(3)	0.2824(4)
y_O	-0.0324(5)	0.0337(5)	0.0352(3)	0.0344(5)
z_O	0.2445(1)	-0.2442(1)	-0.2442(1)	-0.2441(1)
Anisotropic thermal parameters				
Ca site				
U_{11}	0.0123(5)	0.0150(5)	0.0115(3)	0.0159(4)
U_{22}	0.0123(5)	0.0150(5)	0.0115(3)	0.0159(4)
U_{33}	0.0129(7)	0.0178(7)	0.0106(5)	0.0166(6)
U_{23}	0.0	0.0	0.0	0.0
U_{13}	0.0	0.0	0.0	0.0
U_{12}	0.0061(3)	0.0075(3)	0.0058(2)	0.0079(2)
U_{eq}	0.0125(4)	0.0159(5)	0.0112(3)	0.0161(3)
Mg site				
U_{11}	0.0093(8)	0.0124(9)	0.0075(5)	0.0111(4)
U_{22}	0.0093(8)	0.0124(9)	0.0075(5)	0.0111(4)
U_{33}	0.013(1)	0.015(1)	0.0078(8)	0.015(1)
U_{23}	0.0	0.0	0.0	0.0
U_{13}	0.0	0.0	0.0	0.0
U_{12}	0.0047(4)	0.0062(4)	0.0037(3)	0.0055(4)
U_{eq}	0.0105(7)	0.0134(8)	0.0076(4)	0.0124(8)
C				
U_{11}	0.0091(9)	0.0114(9)	0.0087(6)	0.0123(9)
U_{22}	0.0091(9)	0.0114(9)	0.0087(6)	0.0123(9)
U_{33}	0.006(2)	0.011(2)	0.005(1)	0.013(2)
U_{23}	0.0	0.0	0.0	0.0
U_{13}	0.0	0.0	0.0	0.0
U_{12}	0.0046(5)	0.0057(5)	0.0043(3)	0.0061(5)

U_{eq}	0.0079(7)	0.0113(7)	0.0074(5)	0.0125(7)
O				
U_{11}	0.0103(9)	0.0130(8)	0.0078(5)	0.0125(8)
U_{22}	0.018(1)	0.0186(9)	0.0135(6)	0.0181(8)
U_{33}	0.017(1)	0.019(1)	0.0139(7)	0.0205(9)
U_{23}	-0.0009(7)	-0.0011(6)	-0.0025(5)	-0.0025(6)
U_{13}	-0.0013(6)	-0.0004(6)	-0.0007(4)	-0.0003(6)
U_{12}	0.0090(7)	0.0095(7)	0.0059(4)	0.0086(6)
U_{eq}	0.0139(5)	0.0162(5)	0.0115(3)	0.0166(4)
