Supporting information

The crystal structure of calcium sebacate by X-ray powder diffraction data

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Crystallographic data

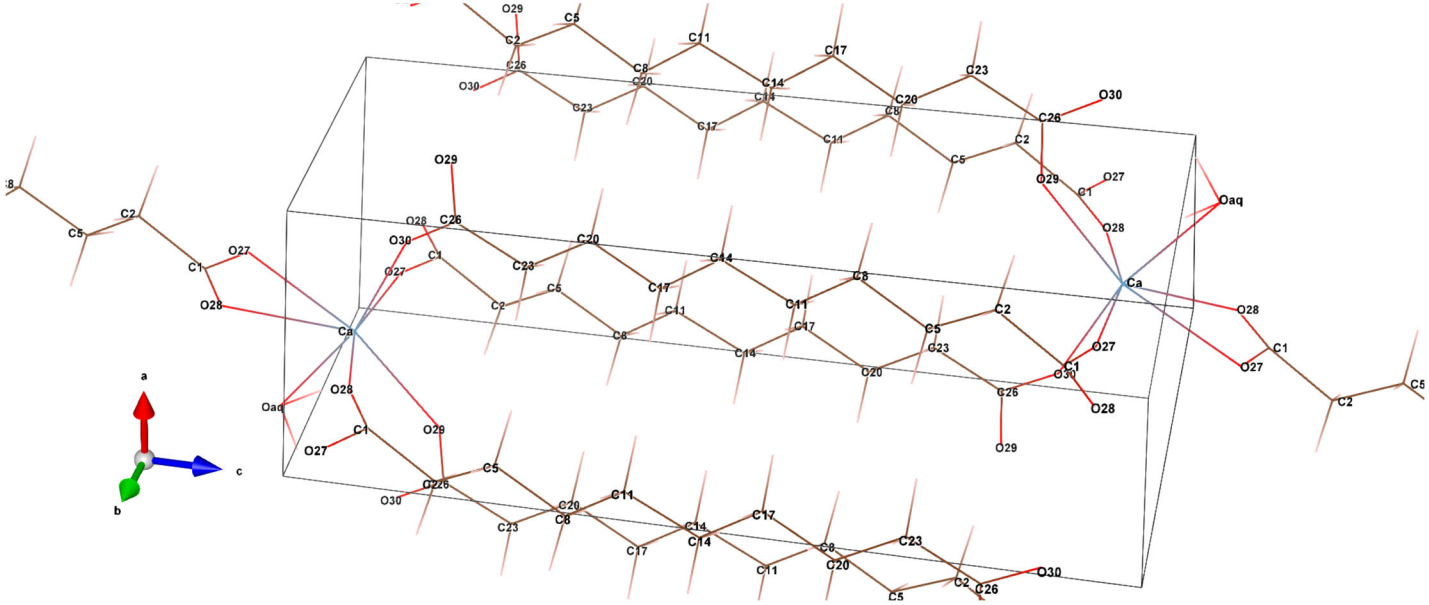


Figure S1. Plot of the calcium sebacate structure with atom labels.

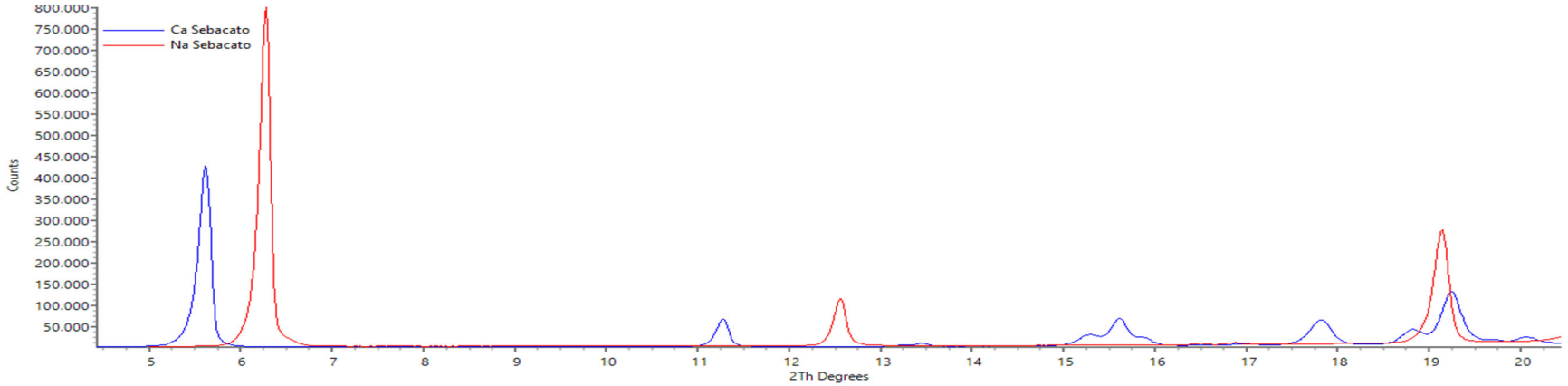
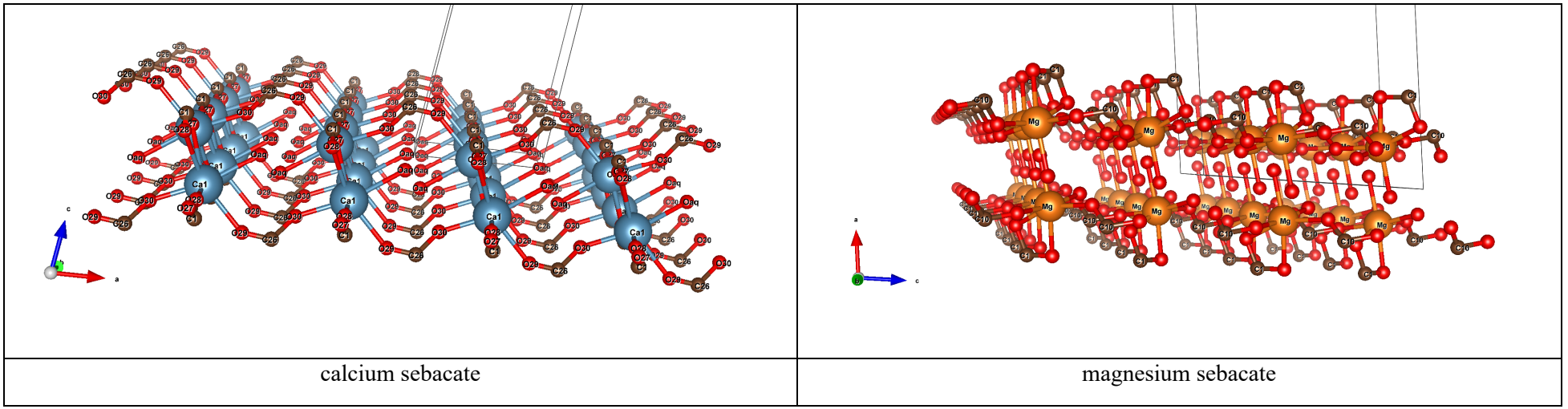


Figure S2. Plot of the XRPD of calcium sebacate vs sodium sebacate



calcium sebacate	magnesium sebacate

Figure S3. Details of Ca coordination and Mg coordination in calcium sebacate vs magnesium sebacate.

Table S1. Crystal data and structure refinement for calcium sebacate.

Compound	Calcium sebacate			
Chemical formula	CaC10H18O5		Z	2
Formula weight/g·mol-1	258.32		Z’	1
Crystal system	triclinic		T/K	293(2)
Space group	P-1		λCu/Å	1.5406
a/Å	5.8633(4)		ρcalc/g·cm^{-3}	1.378
b/Å	6.8363(4)		μ/cm^{-1}	44.106
c/Å	16.059(1)		2θ range/°	4-126°
α/°	79.34(1)		Rp	5.21
β/°	81.318(9)		Rwp	8.832
γ/°	82.834(6)		χ^2	14.065
V/Å3	622.2(1)		CCDC number	2225055

Table S2. Atomic table for the structure of calcium sebacate.

Site	Occupancy	X	Y	Z	Biso	Type
C1	1	0.368(2)	0.1874(13)	0.1190(5)	1.45(17)	C
C2	1	0.196(2)	0.1846(13)	0.2010(5)	1.45(17)	C
H3	1	0.135(2)	0.0525(13)	0.2156(7)	1.45(17)	H
H4	1	0.066(2)	0.2869(13)	0.1895(7)	1.45(17)	H
C5	1	0.316(3)	0.2247(13)	0.2719(5)	1.45(17)	C
H6	1	0.449(3)	0.1219(13)	0.2809(5)	1.45(17)	H
H7	1	0.378(3)	0.3567(13)	0.2549(7)	1.45(17)	H
C8	1	0.160(3)	0.2239(14)	0.3567(5)	1.45(17)	C
H9	1	0.030(3)	0.3298(14)	0.3488(7)	1.45(17)	H
H10	1	0.093(3)	0.0941(14)	0.3730(7)	1.45(17)	H
C11	1	0.305(3)	0.2582(15)	0.4230(7)	1.45(17)	C
H12	1	0.368(3)	0.3889(15)	0.4038(7)	1.45(17)	H
H13	1	0.436(3)	0.1529(15)	0.4267(7)	1.45(17)	H
C14	1	0.170(4)	0.2570(17)	0.5116(5)	1.45(17)	C
H15	1	0.041(4)	0.3652(17)	0.5083(7)	1.45(17)	H
H16	1	0.101(4)	0.1283(17)	0.5300(5)	1.45(17)	H
C17	1	0.317(4)	0.2842(18)	0.5789(7)	1.45(17)	C
H18	1	0.383(4)	0.4140(18)	0.5612(7)	1.45(17)	H
H19	1	0.447(4)	0.1774(18)	0.5812(7)	1.45(17)	H
C20	1	0.166(4)	0.276(2)	0.6637(7)	1.45(17)	C
H21	1	0.041(4)	0.386(2)	0.6593(7)	1.45(17)	H
H22	1	0.095(4)	0.148(2)	0.6771(5)	1.45(17)	H
C23	1	0.296(5)	0.290(2)	0.7368(7)	1.45(17)	C
H24	1	0.427(5)	0.183(2)	0.7393(7)	1.45(17)	H
H25	1	0.636(5)	0.580(2)	0.2756(7)	1.45(17)	H
C26	1	0.147(5)	0.272(2)	0.8230(7)	1.45(17)	C

O27	1	0.408(3)	0.371(2)	0.0848(9)	1.45(17)	O
O28	1	0.398(3)	0.036(2)	0.0821(10)	1.45(17)	O
O29	1	0.062(3)	0.724(2)	0.1685(9)	1.45(17)	O
O30	1	0.267(3)	0.313(2)	0.8841(10)	1.45(17)	O
Oaq	1	0.92689	0.2742	0.03174	3.0(5)	O
H1ac	1	0.05928	0.59546	0.00687	3.0(5)	H
H2ac	1	0.0193	0.1742	0.99963	3.0(5)	H
Ca	1	0.3994(14)	0.7251(9)	0.0594(4)	1.03(15)	Ca

Table S3. Bond distances for the title structure.

Ca:0 O28:1 0 -1 0 2.222(15)

O30:0 -1 1 1 2.24(2) 81.7(7)

O27:1 1 0 0 2.377(15) 87.7(7) 160.9(6)

O29:0 0 1 1 2.44(2) 86.7(7) 112.1(7) 82.6(7)

Oaq:0 0 1 0 2.577(8) 79.4(5) 86.3(5) 166.8(6) 107.1(6)

O27:0 0 1 0 2.58(2) 72.6(5) 148.2(6) 76.8(5) 94.5(8) 119.7(6)

H1ac:0 0 1 0 2.588(7) 78.2(5) 22.13(7) 70.2(4) 66.3(5) 153.9(5) 123.8(7)

H2ac:0 0 1 0 2.727(9) 34.31(11) 91.7(5) 21.27(8) 64.3(5) 99.9(6) 171.1(6) 89.7(6)

O28:0 0 1 0 2.747(15) 89.6(5) 104.6(4) 51.1(5) 85.0(4) 141.5(7) 127.4(7) 89.3(6) 68.6(7)

C1:0 0 1 0 2.969(12) 25.2(4) 89.2(3) 90.5(3) 26.0(3) 76.3(3) 153.2(6) 102.8(5) 93.5(6) 93.8(5)

C1:0 O28:0 0 0 0 1.265(18)

O27:0 0 0 0 1.306(15) 127.2(12)

C2:0 0 0 0 1.52800 110.7(10) 118.7(9)

H3:0 0 0 0 2.06619 27.045 136.3(11) 91.7(9)

H4:0 0 0 0 2.06655 45.451 26.995 91.5(12) 126.0(11)

C5:0 0 0 0 2.48424 53.435 53.501 34.785 98.6(8) 132.7(7)

H6:0 0 0 0 2.65962 21.851 73.624 59.156 50.460 108.7(7) 116.3(8)

H7:0 0 0 0 2.66302 35.014 21.822 58.898 73.591 50.319 77.2(7) 151.3(8)

Ca:0 0 -1 0 2.969(12) 131.4(2) 142.3(3) 151.8(3) 137.3(3) 154.7(3) 164.3(3) 60.0(9) 67.5(8)

H2ac:0 -1 0 0 3.026(12) 71.8(3) 136.5(3) 145.5(2) 131.5(3) 79.4(3) 86.6(2) 97.3(3) 92.9(10) 64.5(11)

Oaq:0 -1 0 0 3.068(14) 18.69(8) 83.0(3) 117.9(2) 134.1(2) 115.7(2) 62.4(2) 80.0(2) 83.6(2) 85.8(11) 82.3(11)

C26:0 O29:0 0 0 0 1.21(4)

O30:0 0 0 0 1.38(2) 123.6(16)

C23:0 0 0 0 1.51700 110.4(13) 123.3(8)

H25:0 0 0 0 2.06503 26.937 92.4(12) 128.7(9)

H24:0 0 0 0 2.06613 45.483 26.946 98.0(14) 137.9(9)

C20:0 0 0 0 2.53917 51.883 51.889 33.144 143.0(13) 90.6(8)

H22:0 0 0 0 2.70644 21.429 57.930 72.015 49.008 155.9(15) 80.2(9)

H21:0 0 0 0 2.74258 34.095 21.134 71.224 56.453 47.892 145.7(10) 76.4(8)

H2ac:0 0 0 -1 2.799(11) 152.0(7) 139.6(5) 160.6(6) 133.9(6) 147.4(6) 159.7(6) 55.3(8) 75.6(9)

H1ac:0 0 0 -1 3.062(12) 30.72(12) 133.1(4) 150.6(6) 154.2(5) 151.1(6) 128.1(5) 154.9(5) 53.2(11) 70.4(9)

H4:1 1 -1 -1 3.09(3) 64.4(4) 95.0(5) 74.2(4) 107.4(4) 93.5(3) 122.4(5) 77.0(5) 98.3(4) 85.9(11) 71.3(12)

H3:1 0 -2 -1 3.13(3) 120.4(12) 110.5(9) 92.7(7) 72.1(3) 46.9(3) 67.9(3) 90.4(6) 118.8(4) 93.7(4) 141.9(10) 53.8(11)

O27:0 C1:0 0 0 0 1.306(15)

O28:0 0 0 0 2.303(19) 25.9(7)

C2:0 0 0 0 2.335(18) 62.5(6) 37.7(6)

Ca:1 1 0 0 2.377(15) 124.5(10) 168.5(8) 162.3(15)

H4:0 0 0 0 2.47(2) 106.4(9) 23.5(2) 77.5(7) 56.7(9)

Ca:0 0 -1 0 2.58(2) 137.1(6) 103.2(5) 130.3(6) 68.2(6) 93.9(10)

H7:0 0 0 0 2.695(17) 153.6(10) 54.7(4) 91.5(5) 47.6(3) 99.4(6) 74.5(7)

H1ac:1 1 -1 0 2.72(2) 116.1(9) 90.3(5) 78.3(7) 60.6(5) 100.7(9) 110.7(8) 115.5(13)

C5:0 0 0 0 2.975(17) 117.9(9) 19.30(12) 144.5(8) 43.7(3) 109.3(6) 30.0(2) 81.1(6) 55.6(6)

Oaq:0 0 0 0 3.05(2) 106.9(7) 134.5(5) 103.1(7) 53.7(5) 146.6(8) 97.9(6) 123.3(8) 83.2(9) 95.9(14)

O27:1 1 -1 0 3.08(3) 67.1(8) 159.3(7) 68.0(7) 140.3(7) 48.7(5) 146.2(14) 54.5(4) 168.0(12) 116.4(10) 142.4(14)

H3:0 0 0 0 3.143(17) 160.8(9) 119.1(7) 39.7(2) 101.4(7) 58.4(3) 118.2(5) 30.13(18) 135.4(9) 12.13(11) 50.7(6) 27.0(7)

O28:0 C1:0 0 0 0 1.265(18)

Ca:1 0 -1 0 2.222(15) 161.3(12)

O27:0 0 0 0 2.303(19) 171.8(9) 26.9(6)

C2:0 0 0 0 2.41(2) 59.4(7) 128.2(7) 33.8(6)

H3:0 0 0 0 2.45(2) 23.5(2) 82.6(8) 104.8(6) 57.3(9)

H2ac:0 -1 0 0 2.73(2) 86.6(8) 87.4(8) 83.2(8) 93.6(6) 90.8(13)

Ca:0 0 -1 0 2.747(15) 79.8(5) 141.9(8) 119.7(6) 60.6(5) 111.4(7) 87.3(7)

O28:1 0 -2 0 2.83(4) 46.9(4) 83.0(7) 164.4(10) 164.8(11) 107.5(8) 64.5(6) 134.2(10)

O30:1 1 -2 -1 2.92(3) 75.5(9) 105.5(8) 142.5(6) 106.8(7) 118.6(7) 132.4(10) 49.4(5) 126.0(13)

H4:0 0 0 0 2.99(3) 135.4(7) 149.1(11) 110.0(6) 71.2(6) 32.2(3) 17.1(2) 53.8(7) 132.2(8) 34.0(9)

O29:1 0 -2 -1 3.08(2) 80.7(6) 80.6(6) 111.6(7) 151.9(6) 79.3(6) 54.7(5) 78.0(6) 134.4(11) 51.7(5) 111.7(12)

Oaq:0 -1 0 0 3.16(2) 80.8(6) 54.0(5) 156.7(5) 98.7(8) 85.0(5) 17.50(15) 73.0(7) 70.6(7) 71.0(8) 107.5(6) 74.3(12)

O29:0 C26:0 0 0 0 1.21(4)

O30:0 0 0 0 2.28(3) 30.3(8)

C23:0 0 0 0 2.40(3) 61.0(8) 31.9(6)

Ca:0 0 -1 -1 2.44(2) 172.8(8) 111.9(7) 141.4(10)

H3:1 0 -2 -1 2.604(16) 94.6(6) 90.7(8) 123.1(11) 104.2(13)

H21:0 0 0 0 2.724(17) 81.1(5) 138.8(10) 46.9(4) 104.2(9) 78.1(10)

H2ac:0 0 0 -1 2.759(14) 157.3(10) 106.4(5) 63.0(4) 110.9(8) 53.6(5) 79.3(9)

H22:0 0 0 0 2.77(2) 138.3(9) 33.8(2) 51.9(6) 140.8(8) 46.3(4) 104.6(11) 74.4(10)

C20:0 0 0 0 2.82(2) 20.34(15) 141.0(10) 20.44(15) 72.2(6) 154.5(9) 32.5(3) 93.5(10) 64.1(9)

H1ac:0 0 0 -1 2.891(14) 145.8(7) 160.8(10) 32.23(15) 143.1(5) 135.4(5) 57.4(4) 115.5(7) 56.2(6) 86.4(8)

H4:1 1 -1 -1 2.940(16) 68.5(4) 91.3(5) 110.1(5) 99.4(4) 77.1(5) 153.6(8) 92.0(7) 85.2(6) 77.2(6) 85.8(11)

H25:0 0 0 0 2.97(3) 68.1(6) 104.3(5) 41.5(4) 59.5(5) 109.2(7) 48.5(4) 107.5(7) 157.9(6) 17.4(2) 55.7(6) 32.8(7)

H24:0 0 0 0 3.07(3) 30.6(3) 98.4(6) 113.0(7) 40.6(4) 47.7(5) 100.5(7) 58.6(5) 82.6(7) 161.9(8) 15.5(2) 56.8(8) 26.8(6)

O28:1 0 -2 -1 3.08(2) 125.4(8) 155.5(9) 136.3(10) 90.6(5) 121.7(6) 101.6(6) 73.6(4) 124.4(7) 50.3(5) 45.7(5) 138.1(9) 123.3(7) 132.5(13)

H7:1 1 -1 -1 3.16(2) 105.1(8) 117.8(5) 91.9(6) 45.8(3) 98.7(6) 84.3(6) 92.5(6) 129.1(7) 63.9(7) 110.5(7) 80.0(7) 102.6(6) 122.7(6) 122.2(10)

O30:0 C26:0 0 0 0 1.38(2)

Ca:0 1 -1 -1 2.24(2) 148.4(18)

O29:0 0 0 0 2.28(3) 167.4(9) 26.2(12)

H2ac:0 0 0 -1 2.310(17) 73.9(7) 101.1(6) 95.4(12)

C23:0 0 0 0 2.378(18) 130.3(8) 62.0(9) 116.8(12) 36.7(6)

H1ac:0 0 0 -1 2.49(2) 133.8(11) 38.0(3) 74.4(8) 109.1(6) 100.5(15)

H25:0 0 0 0 2.53(2) 134.4(10) 23.01(19) 149.8(9) 76.2(8) 107.3(10) 54.7(7)

H24:0 0 0 0 2.64(2) 35.9(3) 151.2(9) 22.0(2) 129.8(7) 76.9(8) 98.7(10) 50.8(8)

Oaq:0 0 0 -1 2.85(2) 145.3(7) 148.8(11) 19.94(14) 138.1(10) 18.53(18) 76.3(7) 102.8(6) 101.4(14)

O28:1 1 -2 -1 2.92(3) 104.0(6) 70.9(7) 101.9(9) 122.7(7) 92.7(9) 88.9(6) 118.8(7) 48.8(5) 105.4(13)

H1ac:1 2 -1 -1 3.03(2) 126.7(6) 47.2(3) 160.1(7) 124.2(7) 32.2(2) 139.9(9) 65.2(5) 98.6(10) 89.5(5) 121.9(16)

Oaq:0 H2ac:0 0 0 0 0.99019

H1ac:0 0 0 0 0.99166 105.099

H1ac:1 2 -1 0 2.36485 32.372 116.496

Ca:0 0 -1 0 2.577(8) 109.80(12) 79.56(11) 87.93(19)

H4:0 1 0 0 2.794(10) 149.6(4) 78.56(16) 110.58(16) 115.1(3)

O30:0 0 0 1 2.85(2) 118.1(4) 91.9(4) 70.4(3) 59.1(4) 47.9(3)

O27:0 0 0 0 3.05(2) 140.8(5) 96.4(4) 53.7(3) 101.5(2) 93.0(3) 133.9(2)

C1:0 1 0 0 3.068(14) 137.0(3) 80.5(4) 40.95(17) 166.1(3) 78.73(14) 105.88(14) 78.3(2)

O28:0 1 0 0 3.16(2) 23.4(3) 147.1(4) 71.5(5) 60.0(4) 142.8(3) 96.0(2) 115.9(2) 56.0(3)

H2ac:1 1 -2 0 3.16731 67.4(2) 89.72(16) 104.9(2) 81.6(3) 109.67(19) 77.58(15) 151.025 133.360 34.568

H1ac:0 Oaq:0 0 0 0 0.99166

H2ac:0 0 0 0 1.57335 37.418

H1ac:1 2 -1 0 1.61696 134.595 128.458

Oaq:1 2 -1 0 2.36485 19.169 144.400 147.628

O30:0 0 0 1 2.49(2) 87.2(3) 92.6(3) 64.6(3) 101.0(4)

Ca:0 0 -1 0 2.588(7) 100.5(4) 131.37(15) 147.39(17) 77.69(18) 78.31(13)

O27:1 1 -1 0 2.72(2) 53.1(3) 110.2(6) 79.0(3) 94.3(3) 129.6(3) 125.4(3)

O29:0 0 0 1 2.891(14) 72.1(6) 52.4(4) 49.4(6) 109.5(2) 125.9(2) 69.2(3) 99.2(3)

H2ac:1 2 -1 0 2.94319 120.8(3) 72.6(3) 125.22(17) 104.7(3) 17.524 22.375 156.970 140.019

O30:1 2 -1 -1 3.03(2) 45.4(3) 148.0(6) 75.9(5) 107.4(4) 147.8(2) 62.4(3) 55.2(3) 136.6(3) 100.1(3)

C26:0 0 0 1 3.062(12) 158.1(4) 114.8(3) 23.1(7) 89.5(6) 75.0(5) 26.3(6) 99.1(4) 110.9(4) 65.3(3) 101.8(3)

H2ac:0 Oaq:0 0 0 0 0.99019

H1ac:0 0 0 0 1.57335 37.483

O30:0 0 0 1 2.310(17) 77.4(5) 113.6(5)

H2ac:1 1 -2 0 2.41810 113.0(4) 157.026 131.997

Ca:0 0 -1 0 2.727(9) 89.46(11) 101.4(5) 68.00(11) 70.80(14)

O28:0 1 0 0 2.73(2) 170.2(3) 85.6(3) 88.3(6) 115.9(3) 106.5(4)

O29:0 0 0 1 2.759(14) 135.8(6) 52.7(5) 91.6(3) 52.5(6) 78.5(4) 107.8(4)

C26:0 0 0 1 2.799(11) 25.1(7) 111.3(7) 77.6(6) 95.9(3) 29.4(6) 83.9(3) 120.2(3)

H1ac:1 2 -1 0 2.94319 86.6(3) 90.6(3) 93.6(3) 90.94(11) 177.477 69.4(4) 23.030 45.981

C1:0 1 0 0 3.026(12) 71.50(17) 119.3(7) 143.2(4) 24.7(4) 153.7(3) 107.26(16) 90.7(5) 92.55(19) 83.0(2)

Oaq:1 1 -2 0 3.16731 105.34(19) 168.511 85.5(3) 85.7(3) 81.6(3) 95.49(12) 13.435 100.0(4) 161.986 145.432

Table S4. BVS and GII calculated for Ca and coordinating oxygen atoms

BVS paramenters were computed both manually and using software as EXPO and VESTA: all calculation methods gave very similar results (a). Noteworthy, manual calculations allowed to perform the bond valence sum method using different bond-valence parameters (bu,bt,bs,o) as detailed in the below reported table.

Computation was performed using bvparm2020.cif: 2020 version

Atom	Atom	Refined distances
Ca	O28:1	2.22
	O30:0	2.24
	O27:1	2.38
	O29:0	2.44
	O27:0	2.58
	O28:0	2.75
	Oaq:0	2.58

Sij	**a**	**bu**	**bt**	**bs**	**o**
	0.504704	0.456675	0.460393	0.465203	0.453734
	0.478147	0.432645	0.436167	0.443002	0.432132
	0.327517	0.296349	0.298762	0.314592	0.307129
	0.278489	0.251987	0.254038	0.271667	0.265317
	0.190757	0.172604	0.174009	0.192921	0.188569
	0.120487	0.109021	0.109908	0.127311	0.124565
	0.190757	0.172604	0.174009	0.192921	0.188569
V Ca	**2.090856**	**1.891884**	**1.907286**	**2.007616**	**1.960015**
G Ca-O	**0.090856**	**0.108116**	**0.092714**	**0.007616**	**0.039985**

Source of used parameters

a from https://scripts.iucr.org/cgi-bin/paper?S0108768185002063 access on 1 February 2023

bu from http://scripts.iucr.org/cgi-bin/paper?S2059798317000584 access on 1 February 2023

bt from https://www.sciencedirect.com/science/article/abs/pii/S0022459618305188 access on 1 February 2023

bs from https://scripts.iucr.org/cgi-bin/paper?yb5007 access on 1 February 2023

o from https://link.springer.com/article/10.1007/BF00902183 access on 1 February 2023

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