

Supporting information for

A phospho-silicate compound, NaCa₃PSiO₈: Structure solution and luminescence properties

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Table S1 Atomic bond distances of the NaCa₃PSiO₈ structure. The numbers in the parenthesis indicates the standard deviation of the least significant figures.

atoms	bond distance (Å)	atoms	bond distance (Å)
Na—Ca1 ⁱ	3.693 (16)	Ca3—O2 ^v	2.26 (2)
Na—Ca1 ⁱⁱ	3.896 (16)	Ca3—O3 ^{xviii}	2.33 (3)
Na—Ca2 ⁱⁱⁱ	3.716 (16)	Ca3—O4 ^{xxi}	2.61 (2)
Na—Ca2 ^{iv}	3.680 (14)	Ca3—O5 ^v	2.74 (2)
Na—Ca2 ^v	3.354 (11)	Ca3—O6	2.36 (2)
Na—Ca3 ^{iv}	3.419 (11)	Ca3—O7 ^v	2.78 (3)
Na—Ca3 ^{vi}	3.728 (18)	Ca3—O7 ^{xviii}	3.26 (2)
Na—Ca3 ^{vii}	3.83 (2)	Ca3—O8 ^x	2.56 (3)
Na—P	3.410 (11)	P—Na	3.410 (11)
Na—P ⁱ	3.015 (16)	P—Na ^{ix}	3.191 (16)
Na—P ⁱⁱ	3.191 (16)	P—Na ^{viii}	3.015 (16)
Na—Si ^{iv}	3.019 (15)	P—Ca1	3.013 (11)
Na—O2	2.72 (3)	P—Ca2 ⁱⁱⁱ	3.466 (13)
Na—O2 ⁱⁱ	2.79 (3)	P—Ca2 ^{iv}	3.265 (13)
Na—O3	2.68 (3)	P—Ca3 ^{xxii}	2.998 (12)
Na—O3 ⁱ	2.85 (3)	P—O1 ^{viii}	1.60 (2)
Na—O4 ⁱ	3.08 (2)	P—O2	1.78 (2)
Na—O4 ⁱⁱ	2.40 (2)	P—O3	1.63 (2)
Na—O5 ^{iv}	2.73 (2)	P—O4	1.361 (18)
Na—O6 ^{iv}	2.49 (2)	Si—Na ^{xiv}	3.019 (15)
Na—O7	2.275 (17)	Si—Ca1	2.992 (10)
Na—O8 ^{viii}	3.00 (3)	Si—Ca1 ^v	3.386 (17)
Ca1—Na ^{ix}	3.896 (16)	Si—Ca1 ^{xviii}	3.186 (16)
Ca1—Na ^{viii}	3.693 (16)	Si—Ca2 ^v	3.082 (11)
Ca1—Ca2	3.744 (12)	Si—Ca3 ^{vi}	3.253 (18)
Ca1—Ca2 ^x	3.586 (12)	Si—Ca3 ^{vii}	3.385 (16)
Ca1—Ca2 ^{vi}	3.745 (9)	Si—O5	1.45 (3)
Ca1—Ca3 ^{xi}	3.559 (10)	Si—O6	1.74 (2)
Ca1—Ca3 ^{vi}	3.624 (14)	Si—O7	1.540 (17)
Ca1—Ca3 ^{vii}	3.516 (14)	Si—O8 ^{vi}	1.48 (3)
Ca1—P	3.013 (11)	O1—Ca1 ^v	2.29 (2)
Ca1—Si	2.992 (10)	O1—Ca2 ^v	2.78 (3)
Ca1—Si ^{vi}	3.386 (17)	O1—Ca3 ^{vi}	2.36 (2)
Ca1—Si ^{vii}	3.186 (16)	O1—P ⁱ	1.60 (2)
Ca1—O1 ^{vi}	2.29 (2)	O2—Na	2.72 (3)
Ca1—O3	3.13 (2)	O2—Na ^{ix}	2.79 (3)
Ca1—O4	2.71 (2)	O2—Ca2 ⁱⁱⁱ	2.33 (3)
Ca1—O5	3.04 (2)	O2—Ca3 ^{vi}	2.26 (2)
Ca1—O5 ^{vi}	2.67 (2)	O2—P	1.78 (2)
Ca1—O6 ^{vi}	2.82 (3)	O3—Na	2.68 (3)
Ca1—O6 ^{vii}	2.66 (3)	O3—Na ^{viii}	2.85 (3)

atoms	bond distance (Å)	atoms	bond distance (Å)
Ca1—O8 ^{xii}	2.67 (3)	O3—Ca1	3.13 (2)
Ca1—O8 ^{vi}	2.71 (3)	O3—Ca2 ^{iv}	2.36 (3)
Ca2—Na ^{xiii}	3.716 (16)	O3—Ca3 ^{vii}	2.33 (3)
Ca2—Na ^{xiv}	3.680 (14)	O3—P	1.63 (2)
Ca2—Na ^{vi}	3.354 (11)	O4—Na ^{ix}	2.40 (2)
Ca2—Ca1 ^{xv}	3.586 (12)	O4—Na ^{viii}	3.08 (2)
Ca2—Ca1	3.744 (12)	O4—Ca1	2.71 (2)
Ca2—Ca1 ^v	3.745 (9)	O4—Ca2 ^{vi}	2.676 (17)
Ca2—Ca3 ^{xvi}	3.451 (13)	O4—Ca3 ^{xxii}	2.61 (2)
Ca2—Ca3 ^{vi}	3.545 (13)	O4—P	1.361 (18)
Ca2—P ^{xiii}	3.466 (13)	O5—Na ^{xiv}	2.73 (2)
Ca2—P ^{xiv}	3.265 (13)	O5—Ca1	3.04 (2)
Ca2—Si ^{vi}	3.082 (11)	O5—Ca1 ^v	2.67 (2)
Ca2—O1 ^{vi}	2.78 (3)	O5—Ca2	2.41 (3)
Ca2—O2 ^{xiii}	2.33 (3)	O5—Ca3 ^{vi}	2.74 (2)
Ca2—O3 ^{xiv}	2.36 (3)	O5—Si	1.45 (3)
Ca2—O4 ^v	2.676 (17)	O6—Na ^{xiv}	2.49 (2)
Ca2—O5	2.41 (3)	O6—Ca1 ^v	2.82 (3)
Ca2—O6 ^{vi}	2.57 (2)	O6—Ca1 ^{xviii}	2.66 (3)
Ca2—O7 ^{vi}	2.51 (2)	O6—Ca2 ^v	2.57 (2)
Ca2—O8 ^{xvii}	2.46 (3)	O6—Ca3	2.36 (2)
Ca3—Na ^{xiv}	3.419 (11)	O6—Si	1.74 (2)
Ca3—Na ^v	3.728 (18)	O7—Na	2.275 (17)
Ca3—Na ^{xviii}	3.83 (2)	O7—Ca2 ^v	2.51 (2)
Ca3—Ca1 ^{xix}	3.559 (10)	O7—Ca3 ^{vi}	2.78 (3)
Ca3—Ca1 ^v	3.624 (14)	O7—Ca3 ^{vii}	3.26 (2)
Ca3—Ca1 ^{xviii}	3.516 (14)	O7—Si	1.540 (17)
Ca3—Ca2 ^{xx}	3.451 (13)	O8—Na ⁱ	3.00 (3)
Ca3—Ca2 ^v	3.545 (13)	O8—Ca1 ^{xxiii}	2.67 (3)
Ca3—P ^{xxi}	2.998 (12)	O8—Ca1 ^v	2.71 (3)
Ca3—Si ^v	3.253 (18)	O8—Ca2 ^{xxiv}	2.46 (3)
Ca3—Si ^{xviii}	3.385 (16)	O8—Ca3 ^{xv}	2.56 (3)
Ca3—O1 ^v	2.36 (2)	O8—Si ^v	1.48 (3)

symmetry codes: (i) $-x+3/2, y-1/2, z+1/2$; (ii) $-x+3/2, y+1/2, z+1/2$; (iii) $x+1/2, -y+1/2, z$; (iv) $x+1/2, -y+3/2, z$; (v) $-x+1, -y+1, z+1/2$; (vi) $-x+1, -y+1, z-1/2$; (vii) $-x+1, -y+2, z-1/2$; (viii) $-x+3/2, y+1/2, z-1/2$; (ix) $-x+3/2, y-1/2, z-1/2$; (x) $x, y+1, z$; (xi) $x, y, z-1$; (xii) $x, y+1, z-1$; (xiii) $x-1/2, -y+1/2, z$; (xiv) $x-1/2, -y+3/2, z$; (xv) $x, y-1, z$; (xvi) $-x+1/2, y-1/2, z-1/2$; (xvii) $-x+1, -y, z-1/2$; (xviii) $-x+1, -y+2, z+1/2$; (xix) $x, y, z+1$; (xx) $-x+1/2, y+1/2, z+1/2$; (xxi) $x-1/2, -y+3/2, z+1$; (xxii) $x+1/2, -y+3/2, z-1$; (xxiii) $x, y-1, z+1$; (xxiv) $-x+1, -y, z+1/2$.

Table S2 Atomic bond angles of the NaCa₃PSiO₈ structure. The numbers in the parenthesis indicate the standard deviation of the least significant figures.

atoms	bond angle (°)	atoms	bond angle (°)
Ca1 ⁱ —Na—Ca2 ⁱⁱⁱ	60.7 (3)	Ca3 ^{xvi} —Ca2—Si ^{vi}	132.3 (3)
Ca1 ⁱ —Na—Ca2 ^{iv}	123.5 (3)	Ca3 ^{xvi} —Ca2—O1 ^{vi}	98.3 (6)
Ca1 ⁱ —Na—Ca2 ^v	99.1 (3)	Ca3 ^{xvi} —Ca2—O2 ^{xiii}	40.4 (5)
Ca1 ⁱ —Na—Ca3 ^{iv}	59.1 (3)	Ca3 ^{xvi} —Ca2—O3 ^{xiv}	42.3 (7)
Ca1 ⁱ —Na—Ca3 ^{vi}	89.7 (5)	Ca3 ^{xvi} —Ca2—O4 ^v	48.4 (4)
Ca1 ⁱ —Na—Ca3 ^{vii}	177.5 (5)	Ca3 ^{xvi} —Ca2—O5	110.3 (5)
Ca1 ⁱ —Na—P ⁱ	52.2 (3)	Ca3 ^{xvi} —Ca2—O6 ^{vi}	166.6 (6)
Ca1 ⁱ —Na—Si ^{iv}	55.6 (4)	Ca3 ^{xvi} —Ca2—O7 ^{vi}	102.9 (5)
Ca1 ⁱ —Na—O2	97.2 (7)	Ca3 ^{xvi} —Ca2—O8 ^{xvii}	115.0 (6)
Ca1 ⁱ —Na—O2 ⁱⁱ	100.0 (5)	Ca3 ^{vi} —Ca2—Si ^{vi}	76.0 (2)
Ca1 ⁱ —Na—O3	143.2 (6)	Ca3 ^{vi} —Ca2—O1 ^{vi}	97.0 (5)
Ca1 ⁱ —Na—O4 ⁱⁱ	135.4 (6)	Ca3 ^{vi} —Ca2—O2 ^{xiii}	140.2 (7)
Ca1 ⁱ —Na—O5 ^{iv}	84.1 (6)	Ca3 ^{vi} —Ca2—O3 ^{xiv}	139.3 (8)
Ca1 ⁱ —Na—O6 ^{iv}	46.1 (6)	Ca3 ^{vi} —Ca2—O4 ^v	103.7 (5)
Ca1 ⁱ —Na—O7	124.4 (8)	Ca3 ^{vi} —Ca2—O5	50.5 (5)
Ca2 ⁱⁱⁱ —Na—Ca2 ^{iv}	95.5 (3)	Ca3 ^{vi} —Ca2—O6 ^{vi}	41.7 (5)
Ca2 ⁱⁱⁱ —Na—Ca2 ^v	129.3 (5)	Ca3 ^{vi} —Ca2—O7 ^{vi}	105.5 (5)
Ca2 ⁱⁱⁱ —Na—Ca3 ^{iv}	119.8 (5)	Ca3 ^{vi} —Ca2—O8 ^{xvii}	46.3 (6)
Ca2 ⁱⁱⁱ —Na—Ca3 ^{vi}	55.2 (3)	Si ^{vi} —Ca2—O1 ^{vi}	63.5 (5)
Ca2 ⁱⁱⁱ —Na—Ca3 ^{vii}	120.5 (3)	Si ^{vi} —Ca2—O2 ^{xiii}	109.5 (7)
Ca2 ⁱⁱⁱ —Na—P ⁱ	71.0 (3)	Si ^{vi} —Ca2—O3 ^{xiv}	111.1 (7)
Ca2 ⁱⁱⁱ —Na—Si ^{iv}	69.1 (4)	Si ^{vi} —Ca2—O4 ^v	173.5 (6)
Ca2 ⁱⁱⁱ —Na—O2	38.6 (5)	Si ^{vi} —Ca2—O5	108.0 (6)
Ca2 ⁱⁱⁱ —Na—O2 ⁱⁱ	159.9 (6)	Si ^{vi} —Ca2—O6 ^{vi}	34.3 (5)
Ca2 ⁱⁱⁱ —Na—O3	85.8 (6)	Si ^{vi} —Ca2—O7 ^{vi}	29.8 (4)
Ca2 ⁱⁱⁱ —Na—O4 ⁱⁱ	142.0 (5)	Si ^{vi} —Ca2—O8 ^{xvii}	100.6 (7)
Ca2 ⁱⁱⁱ —Na—O5 ^{iv}	85.0 (6)	O1 ^{vi} —Ca2—O2 ^{xiii}	121.2 (9)
Ca2 ⁱⁱⁱ —Na—O6 ^{iv}	92.7 (6)	O1 ^{vi} —Ca2—O3 ^{xiv}	57.1 (7)
Ca2 ⁱⁱⁱ —Na—O7	102.2 (8)	O1 ^{vi} —Ca2—O4 ^v	110.3 (7)
Ca2 ^{iv} —Na—Ca2 ^v	130.6 (5)	O1 ^{vi} —Ca2—O5	77.7 (8)
Ca2 ^{iv} —Na—Ca3 ^{iv}	118.1 (5)	O1 ^{vi} —Ca2—O6 ^{vi}	75.9 (8)
Ca2 ^{iv} —Na—Ca3 ^{vi}	119.2 (3)	O1 ^{vi} —Ca2—O7 ^{vi}	55.2 (6)
Ca2 ^{iv} —Na—Ca3 ^{vii}	54.7 (3)	O1 ^{vi} —Ca2—O8 ^{xvii}	143.3 (8)
Ca2 ^{iv} —Na—P ⁱ	166.3 (4)	O2 ^{xiii} —Ca2—O3 ^{xiv}	77.3 (6)
Ca2 ^{iv} —Na—Si ^{iv}	68.3 (4)	O2 ^{xiii} —Ca2—O4 ^v	75.0 (8)
Ca2 ^{iv} —Na—O2	85.4 (5)	O2 ^{xiii} —Ca2—O5	142.5 (7)
Ca2 ^{iv} —Na—O2 ⁱⁱ	100.5 (7)	O2 ^{xiii} —Ca2—O6 ^{vi}	132.8 (9)
Ca2 ^{iv} —Na—O3	39.8 (6)	O2 ^{xiii} —Ca2—O7 ^{vi}	89.4 (9)
Ca2 ^{iv} —Na—O4 ⁱⁱ	46.6 (5)	O2 ^{xiii} —Ca2—O8 ^{xvii}	94.9 (9)
Ca2 ^{iv} —Na—O5 ^{iv}	40.9 (6)	O3 ^{xiv} —Ca2—O4 ^v	64.8 (7)

atoms	bond angle (°)	atoms	bond angle (°)
Ca2 ^{iv} —Na—O6 ^{iv}	90.5 (7)	O3 ^{xiv} —Ca2—O5	90.8 (9)
Ca2 ^{iv} —Na—O7	109.9 (7)	O3 ^{xiv} —Ca2—O6 ^{vi}	132.9 (10)
Ca2 ^v —Na—Ca3 ^{iv}	61.3 (3)	O3 ^{xiv} —Ca2—O7 ^{vi}	85.6 (8)
Ca2 ^v —Na—Ca3 ^{vi}	81.0 (3)	O3 ^{xiv} —Ca2—O8 ^{xvii}	148.3 (9)
Ca2 ^v —Na—Ca3 ^{vii}	81.8 (3)	O4 ^v —Ca2—O5	67.8 (6)
Ca2 ^v —Na—P ⁱ	61.4 (3)	O4 ^v —Ca2—O6 ^{vi}	144.9 (7)
Ca2 ^v —Na—Si ^{iv}	140.0 (3)	O4 ^v —Ca2—O7 ^{vi}	148.8 (7)
Ca2 ^v —Na—O2	115.2 (6)	O4 ^v —Ca2—O8 ^{xvii}	83.4 (7)
Ca2 ^v —Na—O2 ⁱⁱ	43.3 (5)	O5—Ca2—O6 ^{vi}	80.6 (7)
Ca2 ^v —Na—O3	114.7 (6)	O5—Ca2—O7 ^{vi}	125.5 (9)
Ca2 ^v —Na—O4 ⁱⁱ	86.2 (6)	O5—Ca2—O8 ^{xvii}	76.7 (5)
Ca2 ^v —Na—O5 ^{iv}	142.4 (7)	O6 ^{vi} —Ca2—O7 ^{vi}	63.8 (6)
Ca2 ^v —Na—O6 ^{iv}	104.9 (5)	O6 ^{vi} —Ca2—O8 ^{xvii}	74.3 (8)
Ca2 ^v —Na—O7	48.5 (5)	O7 ^{vi} —Ca2—O8 ^{xvii}	125.4 (10)
Ca3 ^{iv} —Na—Ca3 ^{vi}	122.7 (5)	Na ^{xiv} —Ca3—Na ^v	100.9 (4)
Ca3 ^{iv} —Na—Ca3 ^{vii}	119.7 (5)	Na ^{xiv} —Ca3—Na ^{xviii}	98.8 (4)
Ca3 ^{iv} —Na—P ⁱ	72.3 (4)	Na ^{xiv} —Ca3—Ca1 ^{xix}	156.4 (3)
Ca3 ^{iv} —Na—Si ^{iv}	78.8 (3)	Na ^{xiv} —Ca3—Ca1 ^v	67.1 (3)
Ca3 ^{iv} —Na—O2	152.7 (8)	Na ^{xiv} —Ca3—Ca1 ^{xviii}	64.3 (4)
Ca3 ^{iv} —Na—O2 ⁱⁱ	41.1 (5)	Na ^{xiv} —Ca3—Ca2 ^{xx}	58.4 (2)
Ca3 ^{iv} —Na—O3	151.0 (8)	Na ^{xiv} —Ca3—Ca2 ^v	93.2 (2)
Ca3 ^{iv} —Na—O4 ⁱⁱ	86.7 (6)	Na ^{xiv} —Ca3—P ^{xxi}	133.5 (3)
Ca3 ^{iv} —Na—O5 ^{iv}	90.2 (6)	Na ^{xiv} —Ca3—Si ^v	117.8 (4)
Ca3 ^{iv} —Na—O6 ^{iv}	43.7 (5)	Na ^{xiv} —Ca3—O1 ^v	164.3 (7)
Ca3 ^{iv} —Na—O7	109.7 (6)	Na ^{xiv} —Ca3—O2 ^v	54.4 (8)
Ca3 ^{vi} —Na—Ca3 ^{vii}	92.8 (3)	Na ^{xiv} —Ca3—O3 ^{xviii}	55.5 (7)
Ca3 ^{vi} —Na—P ⁱ	51.5 (3)	Na ^{xiv} —Ca3—O4 ^{xxi}	107.8 (5)
Ca3 ^{vi} —Na—Si ^{iv}	124.0 (6)	Na ^{xiv} —Ca3—O5 ^v	117.8 (5)
Ca3 ^{vi} —Na—O2	37.0 (5)	Na ^{xiv} —Ca3—O6	46.8 (5)
Ca3 ^{vi} —Na—O2 ⁱⁱ	124.2 (6)	Na ^{xiv} —Ca3—O7 ^v	117.3 (5)
Ca3 ^{vi} —Na—O3	82.2 (6)	Na ^{xiv} —Ca3—O8 ^x	112.1 (8)
Ca3 ^{vi} —Na—O4 ⁱⁱ	134.7 (7)	Na ^v —Ca3—Na ^{xviii}	92.8 (3)
Ca3 ^{vi} —Na—O5 ^{iv}	136.6 (6)	Na ^v —Ca3—Ca1 ^{xix}	98.5 (3)
Ca3 ^{vi} —Na—O6 ^{iv}	135.8 (7)	Na ^v —Ca3—Ca1 ^v	81.1 (4)
Ca3 ^{vi} —Na—O7	47.9 (7)	Na ^v —Ca3—Ca1 ^{xviii}	162.5 (3)
Ca3 ^{vii} —Na—P ⁱ	130.1 (4)	Na ^v —Ca3—Ca2 ^{xx}	62.2 (3)
Ca3 ^{vii} —Na—Si ^{iv}	122.3 (6)	Na ^v —Ca3—Ca2 ^v	132.4 (5)
Ca3 ^{vii} —Na—O2	84.5 (6)	Na ^v —Ca3—P ^{xxi}	51.9 (3)
Ca3 ^{vii} —Na—O2 ⁱⁱ	79.1 (6)	Na ^v —Ca3—Si ^v	65.4 (4)
Ca3 ^{vii} —Na—O3	36.9 (5)	Na ^v —Ca3—O1 ^v	65.3 (6)
Ca3 ^{vii} —Na—O4 ⁱⁱ	42.2 (5)	Na ^v —Ca3—O2 ^v	46.6 (7)
Ca3 ^{vii} —Na—O5 ^{iv}	93.8 (7)	Na ^v —Ca3—O3 ^{xviii}	103.6 (7)
Ca3 ^{vii} —Na—O6 ^{iv}	131.4 (7)	Na ^v —Ca3—O4 ^{xxi}	54.8 (4)
Ca3 ^{vii} —Na—O7	58.0 (7)	Na ^v —Ca3—O5 ^v	91.6 (6)
P ⁱ —Na—Si ^{iv}	107.3 (6)	Na ^v —Ca3—O6	127.9 (8)

atoms	bond angle (°)	atoms	bond angle (°)
P ⁱ —Na—O2	82.5 (6)	Na ^v —Ca3—O7 ^v	37.5 (4)
P ⁱ —Na—O2 ⁱⁱ	93.2 (6)	Na ^v —Ca3—O8 ^x	146.7 (7)
P ⁱ —Na—O3	133.6 (8)	Na ^{xviii} —Ca3—Ca1 ^{xix}	93.6 (2)
P ⁱ —Na—O4 ⁱⁱ	146.9 (6)	Na ^{xviii} —Ca3—Ca1 ^v	163.0 (3)
P ⁱ —Na—O5 ^{iv}	136.1 (8)	Na ^{xviii} —Ca3—Ca1 ^{xviii}	81.1 (4)
P ⁱ —Na—O6 ^{iv}	92.2 (7)	Na ^{xviii} —Ca3—Ca2 ^{xx}	60.4 (3)
P ⁱ —Na—O7	72.2 (7)	Na ^{xviii} —Ca3—Ca2 ^v	129.9 (4)
Si ^{iv} —Na—O2	99.6 (6)	Na ^{xviii} —Ca3—P ^{xxi}	54.1 (3)
Si ^{iv} —Na—O2 ⁱⁱ	105.7 (6)	Na ^{xviii} —Ca3—Si ^v	139.6 (3)
Si ^{iv} —Na—O3	100.4 (7)	Na ^{xviii} —Ca3—O1 ^v	75.5 (6)
Si ^{iv} —Na—O4 ⁱⁱ	92.8 (7)	Na ^{xviii} —Ca3—O2 ^v	101.3 (7)
Si ^{iv} —Na—O5 ^{iv}	28.7 (5)	Na ^{xviii} —Ca3—O3 ^{xviii}	43.5 (6)
Si ^{iv} —Na—O6 ^{iv}	35.1 (6)	Na ^{xviii} —Ca3—O4 ^{xxi}	38.2 (4)
Si ^{iv} —Na—O7	170.4 (8)	Na ^{xviii} —Ca3—O5 ^v	141.6 (5)
O2—Na—O2 ⁱⁱ	154.4 (5)	Na ^{xviii} —Ca3—O6	126.4 (9)
O2—Na—O3	56.3 (5)	Na ^{xviii} —Ca3—O7 ^v	120.0 (5)
O2—Na—O4 ⁱⁱ	120.5 (8)	Na ^{xviii} —Ca3—O8 ^x	87.1 (7)
O2—Na—O5 ^{iv}	101.3 (7)	Ca1 ^{xix} —Ca3—Ca1 ^v	103.0 (2)
O2—Na—O6 ^{iv}	130.0 (8)	Ca1 ^{xix} —Ca3—Ca1 ^{xviii}	98.2 (2)
O2—Na—O7	70.9 (8)	Ca1 ^{xix} —Ca3—Ca2 ^{xx}	144.5 (2)
O2 ⁱⁱ —Na—O3	114.3 (10)	Ca1 ^{xix} —Ca3—Ca2 ^v	63.62 (18)
O2 ⁱⁱ —Na—O4 ⁱⁱ	55.4 (7)	Ca1 ^{xix} —Ca3—P ^{xxi}	69.8 (2)
O2 ⁱⁱ —Na—O5 ^{iv}	99.1 (9)	Ca1 ^{xix} —Ca3—Si ^v	59.4 (3)
O2 ⁱⁱ —Na—O6 ^{iv}	75.2 (7)	Ca1 ^{xix} —Ca3—O1 ^v	39.2 (6)
O2 ⁱⁱ —Na—O7	83.8 (8)	Ca1 ^{xix} —Ca3—O2 ^v	142.0 (9)
O3—Na—O4 ⁱⁱ	64.3 (8)	Ca1 ^{xix} —Ca3—O3 ^{xviii}	131.7 (8)
O3—Na—O5 ^{iv}	77.9 (8)	Ca1 ^{xix} —Ca3—O4 ^{xxi}	94.4 (4)
O3—Na—O6 ^{iv}	129.5 (9)	Ca1 ^{xix} —Ca3—O5 ^v	48.0 (5)
O3—Na—O7	74.4 (8)	Ca1 ^{xix} —Ca3—O6	109.9 (6)
O4 ⁱⁱ —Na—O5 ^{iv}	67.0 (8)	Ca1 ^{xix} —Ca3—O7 ^v	72.2 (4)
O4 ⁱⁱ —Na—O6 ^{iv}	89.5 (8)	Ca1 ^{xix} —Ca3—O8 ^x	48.3 (6)
O4 ⁱⁱ —Na—O7	92.1 (10)	Ca1 ^v —Ca3—Ca1 ^{xviii}	100.1 (3)
O5 ^{iv} —Na—O6 ^{iv}	51.7 (8)	Ca1 ^v —Ca3—Ca2 ^{xx}	102.9 (3)
O5 ^{iv} —Na—O7	150.7 (10)	Ca1 ^v —Ca3—Ca2 ^v	63.0 (3)
O6 ^{iv} —Na—O7	153.2 (8)	Ca1 ^v —Ca3—P ^{xxi}	128.6 (5)
Na ^{viii} —Ca1—Ca2	174.2 (3)	Ca1 ^v —Ca3—Si ^v	51.2 (3)
Na ^{viii} —Ca1—Ca2 ^x	88.1 (3)	Ca1 ^v —Ca3—O1 ^v	115.4 (7)
Na ^{viii} —Ca1—Ca2 ^{vi}	59.9 (2)	Ca1 ^v —Ca3—O2 ^v	63.0 (7)
Na ^{viii} —Ca1—Ca3 ^{xi}	99.1 (2)	Ca1 ^v —Ca3—O3 ^{xviii}	122.4 (7)
Na ^{viii} —Ca1—Ca3 ^{vi}	121.8 (2)	Ca1 ^v —Ca3—O4 ^{xxi}	134.6 (5)
Na ^{viii} —Ca1—Ca3 ^{vii}	56.6 (3)	Ca1 ^v —Ca3—O5 ^v	55.0 (5)
Na ^{viii} —Ca1—P	52.2 (3)	Ca1 ^v —Ca3—O6	51.0 (7)
Na ^{viii} —Ca1—Si	117.4 (4)	Ca1 ^v —Ca3—O7 ^v	63.1 (5)
Na ^{viii} —Ca1—Si ^{vii}	51.4 (3)	Ca1 ^v —Ca3—O8 ^x	106.8 (7)
Na ^{viii} —Ca1—O1 ^{vi}	132.3 (7)	Ca1 ^{xviii} —Ca3—Ca2 ^{xx}	100.8 (3)

atoms	bond angle (°)	atoms	bond angle (°)
Na ^{viii} —Ca1—O4	54.9 (4)	Ca1 ^{xviii} —Ca3—Ca2 ^v	61.0 (2)
Na ^{viii} —Ca1—O5 ^{vi}	99.4 (6)	Ca1 ^{xviii} —Ca3—P ^{xxi}	131.1 (5)
Na ^{viii} —Ca1—O6 ^{vi}	131.9 (5)	Ca1 ^{xviii} —Ca3—Si ^v	128.7 (3)
Na ^{viii} —Ca1—O6 ^{vii}	42.5 (5)	Ca1 ^{xviii} —Ca3—O1 ^v	127.7 (7)
Na ^{viii} —Ca1—O8 ^{xii}	53.4 (5)	Ca1 ^{xviii} —Ca3—O2 ^v	118.4 (8)
Na ^{viii} —Ca1—O8 ^{vi}	101.2 (7)	Ca1 ^{xviii} —Ca3—O3 ^{xviii}	60.8 (7)
Ca2—Ca1—Ca2 ^x	96.6 (2)	Ca1 ^{xviii} —Ca3—O4 ^{xxi}	118.7 (5)
Ca2—Ca1—Ca2 ^{vi}	114.5 (2)	Ca1 ^{xviii} —Ca3—O5 ^v	103.5 (6)
Ca2—Ca1—Ca3 ^{xi}	78.16 (19)	Ca1 ^{xviii} —Ca3—O6	49.2 (7)
Ca2—Ca1—Ca3 ^{vi}	57.5 (3)	Ca1 ^{xviii} —Ca3—O7 ^v	156.7 (5)
Ca2—Ca1—Ca3 ^{vii}	128.9 (3)	Ca1 ^{xviii} —Ca3—O8 ^x	49.9 (6)
Ca2—Ca1—P	125.7 (4)	Ca2 ^{xx} —Ca3—Ca2 ^v	151.53 (17)
Ca2—Ca1—Si	67.6 (3)	Ca2 ^{xx} —Ca3—P ^{xxi}	75.1 (3)
Ca2—Ca1—Si ^{vii}	129.4 (3)	Ca2 ^{xx} —Ca3—Si ^v	124.5 (4)
Ca2—Ca1—O1 ^{vi}	47.7 (6)	Ca2 ^{xx} —Ca3—O1 ^v	106.7 (6)
Ca2—Ca1—O4	120.4 (4)	Ca2 ^{xx} —Ca3—O2 ^v	41.9 (6)
Ca2—Ca1—O5 ^{vi}	74.9 (5)	Ca2 ^{xx} —Ca3—O3 ^{xviii}	42.9 (6)
Ca2—Ca1—O6 ^{vi}	43.3 (5)	Ca2 ^{xx} —Ca3—O4 ^{xxi}	50.1 (4)
Ca2—Ca1—O6 ^{vii}	142.1 (5)	Ca2 ^{xx} —Ca3—O5 ^v	149.6 (6)
Ca2—Ca1—O8 ^{xii}	124.1 (6)	Ca2 ^{xx} —Ca3—O6	105.2 (6)
Ca2—Ca1—O8 ^{vi}	84.5 (6)	Ca2 ^{xx} —Ca3—O7 ^v	98.8 (4)
Ca2 ^x —Ca1—Ca2 ^{vi}	120.1 (3)	Ca2 ^{xx} —Ca3—O8 ^x	141.1 (8)
Ca2 ^x —Ca1—Ca3 ^{xi}	82.6 (2)	Ca2 ^v —Ca3—P ^{xxi}	133.3 (3)
Ca2 ^x —Ca1—Ca3 ^{vi}	128.4 (3)	Ca2 ^v —Ca3—Si ^v	67.8 (3)
Ca2 ^x —Ca1—Ca3 ^{vii}	59.9 (3)	Ca2 ^v —Ca3—O1 ^v	101.7 (6)
Ca2 ^x —Ca1—P	129.0 (4)	Ca2 ^v —Ca3—O2 ^v	124.5 (7)
Ca2 ^x —Ca1—Si	71.3 (3)	Ca2 ^v —Ca3—O3 ^{xviii}	121.4 (7)
Ca2 ^x —Ca1—Si ^{vii}	53.8 (3)	Ca2 ^v —Ca3—O4 ^{xxi}	156.6 (4)
Ca2 ^x —Ca1—O1 ^{vi}	66.6 (6)	Ca2 ^v —Ca3—O5 ^v	42.7 (5)
Ca2 ^x —Ca1—O4	143.0 (4)	Ca2 ^v —Ca3—O6	46.4 (6)
Ca2 ^x —Ca1—O5 ^{vi}	132.4 (5)	Ca2 ^v —Ca3—O7 ^v	96.0 (5)
Ca2 ^x —Ca1—O6 ^{vi}	139.8 (5)	Ca2 ^v —Ca3—O8 ^x	43.9 (7)
Ca2 ^x —Ca1—O6 ^{vii}	45.6 (5)	P ^{xxi} —Ca3—Si ^v	86.9 (4)
Ca2 ^x —Ca1—O8 ^{xii}	79.2 (6)	P ^{xxi} —Ca3—O1 ^v	32.0 (6)
Ca2 ^x —Ca1—O8 ^{vi}	43.2 (6)	P ^{xxi} —Ca3—O2 ^v	91.2 (7)
Ca2 ^{vi} —Ca1—Ca3 ^{xi}	58.0 (2)	P ^{xxi} —Ca3—O3 ^{xviii}	91.4 (6)
Ca2 ^{vi} —Ca1—Ca3 ^{vi}	111.5 (3)	P ^{xxi} —Ca3—O4 ^{xxi}	27.0 (4)
Ca2 ^{vi} —Ca1—Ca3 ^{vii}	116.5 (3)	P ^{xxi} —Ca3—O5 ^v	101.6 (5)
Ca2 ^{vi} —Ca1—P	70.5 (3)	P ^{xxi} —Ca3—O6	180.000 (8)
Ca2 ^{vi} —Ca1—Si	167.0 (4)	P ^{xxi} —Ca3—O7 ^v	66.5 (5)
Ca2 ^{vi} —Ca1—Si ^{vii}	67.2 (3)	P ^{xxi} —Ca3—O8 ^x	104.0 (6)
Ca2 ^{vi} —Ca1—O1 ^{vi}	97.7 (6)	Si ^v —Ca3—O1 ^v	64.6 (6)
Ca2 ^{vi} —Ca1—O4	45.6 (4)	Si ^v —Ca3—O2 ^v	87.9 (8)
Ca2 ^{vi} —Ca1—O5 ^{vi}	39.9 (5)	Si ^v —Ca3—O3 ^{xviii}	167.0 (8)
Ca2 ^{vi} —Ca1—O6 ^{vi}	84.5 (5)	Si ^v —Ca3—O4 ^{xxi}	109.2 (5)

atoms	bond angle (°)	atoms	bond angle (°)
Ca2 ^{vi} —Ca1—O6 ^{vii}	89.3 (6)	Si ^v —Ca3—O5 ^v	26.3 (5)
Ca2 ^{vi} —Ca1—O8 ^{xii}	40.9 (6)	Si ^v —Ca3—O6	92.6 (8)
Ca2 ^{vi} —Ca1—O8 ^{vi}	158.2 (8)	Si ^v —Ca3—O7 ^v	28.2 (4)
Ca3 ^{xi} —Ca1—Ca3 ^{vi}	125.6 (2)	Si ^v —Ca3—O8 ^x	93.9 (7)
Ca3 ^{xi} —Ca1—Ca3 ^{vii}	133.5 (3)	O1 ^v —Ca3—O2 ^v	111.8 (9)
Ca3 ^{xi} —Ca1—P	128.5 (3)	O1 ^v —Ca3—O3 ^{xviii}	118.4 (9)
Ca3 ^{xi} —Ca1—Si	133.3 (3)	O1 ^v —Ca3—O4 ^{xxi}	58.7 (6)
Ca3 ^{xi} —Ca1—Si ^{vii}	60.0 (3)	O1 ^v —Ca3—O5 ^v	71.8 (8)
Ca3 ^{xi} —Ca1—O1 ^{vi}	40.7 (6)	O1 ^v —Ca3—O6	147.6 (9)
Ca3 ^{xi} —Ca1—O4	102.5 (4)	O1 ^v —Ca3—O7 ^v	56.7 (6)
Ca3 ^{xi} —Ca1—O5 ^{vi}	49.7 (5)	O1 ^v —Ca3—O8 ^x	82.5 (8)
Ca3 ^{xi} —Ca1—O6 ^{vi}	85.8 (5)	O2 ^v —Ca3—O3 ^{xviii}	79.2 (6)
Ca3 ^{xi} —Ca1—O6 ^{vii}	92.2 (5)	O2 ^v —Ca3—O4 ^{xxi}	77.5 (7)
Ca3 ^{xi} —Ca1—O8 ^{xii}	45.9 (6)	O2 ^v —Ca3—O5 ^v	109.1 (9)
Ca3 ^{xi} —Ca1—O8 ^{vi}	120.3 (5)	O2 ^v —Ca3—O6	88.8 (10)
Ca3 ^{vi} —Ca1—Ca3 ^{vii}	100.1 (3)	O2 ^v —Ca3—O7 ^v	70.1 (8)
Ca3 ^{vi} —Ca1—P	70.2 (3)	O2 ^v —Ca3—O8 ^x	164.8 (10)
Ca3 ^{vi} —Ca1—Si	58.0 (4)	O3 ^{xviii} —Ca3—O4 ^{xxi}	66.3 (7)
Ca3 ^{vi} —Ca1—Si ^{vii}	173.1 (3)	O3 ^{xviii} —Ca3—O5 ^v	164.2 (8)
Ca3 ^{vi} —Ca1—O1 ^{vi}	105.2 (7)	O3 ^{xviii} —Ca3—O6	89.1 (10)
Ca3 ^{vi} —Ca1—O4	78.4 (4)	O3 ^{xviii} —Ca3—O7 ^v	141.1 (8)
Ca3 ^{vi} —Ca1—O5 ^{vi}	86.8 (5)	O3 ^{xviii} —Ca3—O8 ^x	99.0 (9)
Ca3 ^{vi} —Ca1—O6 ^{vi}	40.7 (5)	O4 ^{xxi} —Ca3—O5 ^v	127.9 (7)
Ca3 ^{vi} —Ca1—O6 ^{vii}	142.1 (6)	O4 ^{xxi} —Ca3—O6	153.5 (8)
Ca3 ^{vi} —Ca1—O8 ^{xii}	152.3 (7)	O4 ^{xxi} —Ca3—O7 ^v	83.8 (6)
Ca3 ^{vi} —Ca1—O8 ^{vi}	87.3 (7)	O4 ^{xxi} —Ca3—O8 ^x	115.9 (7)
Ca3 ^{vii} —Ca1—P	70.9 (3)	O5 ^v —Ca3—O6	77.9 (7)
Ca3 ^{vii} —Ca1—Si	62.1 (3)	O5 ^v —Ca3—O7 ^v	54.1 (6)
Ca3 ^{vii} —Ca1—Si ^{vii}	75.2 (3)	O5 ^v —Ca3—O8 ^x	69.3 (5)
Ca3 ^{vii} —Ca1—O1 ^{vi}	125.6 (7)	O6—Ca3—O7 ^v	113.0 (9)
Ca3 ^{vii} —Ca1—O4	93.9 (4)	O6—Ca3—O8 ^x	76.0 (8)
Ca3 ^{vii} —Ca1—O5 ^{vi}	155.1 (5)	O7 ^v —Ca3—O8 ^x	116.8 (8)
Ca3 ^{vii} —Ca1—O6 ^{vi}	140.6 (5)	Na ^{viii} —P—Ca1	75.6 (4)
Ca3 ^{vii} —Ca1—O6 ^{vii}	42.2 (5)	Na ^{viii} —P—Ca3 ^{xxii}	76.6 (4)
Ca3 ^{vii} —Ca1—O8 ^{xii}	97.1 (6)	Na ^{viii} —P—O1 ^{viii}	92.8 (10)
Ca3 ^{vii} —Ca1—O8 ^{vi}	46.4 (5)	Na ^{viii} —P—O2	155.0 (9)
P—Ca1—Si	97.6 (3)	Na ^{viii} —P—O3	68.3 (10)
P—Ca1—Si ^{vii}	103.3 (4)	Na ^{viii} —P—O4	79.8 (9)
P—Ca1—O1 ^{vi}	163.5 (7)	Ca1—P—Ca3 ^{xxii}	121.1 (3)
P—Ca1—O4	26.9 (4)	Ca1—P—O1 ^{viii}	167.9 (11)
P—Ca1—O5 ^{vi}	89.4 (5)	Ca1—P—O2	82.2 (8)
P—Ca1—O6 ^{vi}	87.5 (5)	Ca1—P—O3	78.7 (9)
P—Ca1—O6 ^{vii}	89.0 (5)	Ca1—P—O4	64.2 (10)
P—Ca1—O8 ^{xii}	95.5 (6)	Ca3 ^{xxii} —P—O1 ^{viii}	51.4 (9)
P—Ca1—O8 ^{vi}	107.9 (6)	Ca3 ^{xxii} —P—O2	125.8 (10)

atoms	bond angle (°)	atoms	bond angle (°)
Si—Ca1—Si ^{vii}	122.3 (3)	Ca3 ^{xxii} —P—O3	133.6 (12)
Si—Ca1—O1 ^{vi}	92.8 (6)	Ca3 ^{xxii} —P—O4	60.4 (10)
Si—Ca1—O4	121.7 (5)	O1 ^{viii} —P—O2	109.8 (11)
Si—Ca1—O5 ^{vi}	138.3 (6)	O1 ^{viii} —P—O3	100.3 (12)
Si—Ca1—O6 ^{vi}	89.9 (6)	O1 ^{viii} —P—O4	111.1 (14)
Si—Ca1—O6 ^{vii}	95.8 (7)	O2—P—O3	96.4 (8)
Si—Ca1—O8 ^{xii}	149.6 (6)	O2—P—O4	100.9 (13)
Si—Ca1—O8 ^{vi}	29.5 (6)	O3—P—O4	135.9 (14)
Si ^{vii} —Ca1—O1 ^{vi}	81.7 (7)	Na ^{xiv} —Si—Ca1	101.8 (4)
Si ^{vii} —Ca1—O4	96.8 (4)	Na ^{xiv} —Si—Ca1 ^{xviii}	73.0 (4)
Si ^{vii} —Ca1—O5 ^{vi}	95.4 (5)	Na ^{xiv} —Si—Ca2 ^v	112.0 (3)
Si ^{vii} —Ca1—O6 ^{vi}	143.4 (6)	Na ^{xiv} —Si—Ca3 ^{vi}	121.0 (6)
Si ^{vii} —Ca1—O6 ^{vii}	33.0 (5)	Na ^{xiv} —Si—O5	64.4 (9)
Si ^{vii} —Ca1—O8 ^{xii}	27.4 (6)	Na ^{xiv} —Si—O6	55.7 (8)
Si ^{vii} —Ca1—O8 ^{vi}	92.8 (7)	Na ^{xiv} —Si—O7	164.6 (10)
O1 ^{vi} —Ca1—O4	137.8 (7)	Na ^{xiv} —Si—O8 ^{vi}	75.1 (10)
O1 ^{vi} —Ca1—O5 ^{vi}	74.3 (7)	Ca1—Si—Ca1 ^{xviii}	120.0 (5)
O1 ^{vi} —Ca1—O6 ^{vi}	79.7 (7)	Ca1—Si—Ca2 ^v	146.0 (4)
O1 ^{vi} —Ca1—O6 ^{vii}	102.8 (8)	Ca1—Si—Ca3 ^{vi}	70.8 (3)
O1 ^{vi} —Ca1—O8 ^{xii}	81.6 (8)	Ca1—Si—O5	78.0 (9)
O1 ^{vi} —Ca1—O8 ^{vi}	87.4 (7)	Ca1—Si—O6	157.5 (9)
O4—Ca1—O5 ^{vi}	63.8 (6)	Ca1—Si—O7	92.5 (9)
O4—Ca1—O6 ^{vi}	77.2 (6)	Ca1—Si—O8 ^{vi}	64.5 (10)
O4—Ca1—O6 ^{vii}	97.4 (6)	Ca1 ^{xviii} —Si—Ca2 ^v	69.8 (3)
O4—Ca1—O8 ^{xii}	78.9 (7)	Ca1 ^{xviii} —Si—Ca3 ^{vi}	161.9 (4)
O4—Ca1—O8 ^{vi}	134.7 (6)	Ca1 ^{xviii} —Si—O5	136.6 (9)
O5 ^{vi} —Ca1—O6 ^{vi}	49.2 (6)	Ca1 ^{xviii} —Si—O6	56.7 (11)
O5 ^{vi} —Ca1—O6 ^{vii}	125.5 (8)	Ca1 ^{xviii} —Si—O7	104.8 (11)
O5 ^{vi} —Ca1—O8 ^{xii}	68.9 (5)	Ca1 ^{xviii} —Si—O8 ^{vi}	56.3 (11)
O5 ^{vi} —Ca1—O8 ^{vi}	158.5 (7)	Ca2 ^v —Si—Ca3 ^{vi}	93.3 (4)
O6 ^{vi} —Ca1—O6 ^{vii}	173.6 (10)	Ca2 ^v —Si—O5	118.9 (12)
O6 ^{vi} —Ca1—O8 ^{xii}	118.0 (9)	Ca2 ^v —Si—O6	56.4 (8)
O6 ^{vi} —Ca1—O8 ^{vi}	117.3 (9)	Ca2 ^v —Si—O7	54.2 (8)
O6 ^{vii} —Ca1—O8 ^{xii}	57.1 (7)	Ca2 ^v —Si—O8 ^{vi}	121.0 (13)
O6 ^{vii} —Ca1—O8 ^{vi}	68.9 (8)	Ca3 ^{vi} —Si—O5	56.8 (9)
O8 ^{xii} —Ca1—O8 ^{vi}	120.1 (3)	Ca3 ^{vi} —Si—O6	119.4 (13)
Na ^{xiii} —Ca2—Na ^{xiv}	95.5 (3)	Ca3 ^{vi} —Si—O7	58.5 (11)
Na ^{xiii} —Ca2—Na ^{vi}	102.4 (3)	Ca3 ^{vi} —Si—O8 ^{vi}	134.9 (10)
Na ^{xiii} —Ca2—Ca1 ^{xv}	79.4 (3)	O5—Si—O6	91.1 (15)
Na ^{xiii} —Ca2—Ca1	155.6 (2)	O5—Si—O7	114.0 (16)
Na ^{xiii} —Ca2—Ca1 ^v	59.3 (2)	O5—Si—O8 ^{vi}	116.4 (10)
Na ^{xiii} —Ca2—Ca3 ^{xvi}	62.6 (3)	O6—Si—O7	110.0 (12)
Na ^{xiii} —Ca2—Ca3 ^{vi}	98.9 (3)	O6—Si—O8 ^{vi}	104.5 (17)
Na ^{xiii} —Ca2—Si ^{vi}	131.7 (4)	O7—Si—O8 ^{vi}	116.9 (15)
Na ^{xiii} —Ca2—O1 ^{vi}	160.5 (6)	Ca1 ^v —O1—Ca2 ^v	94.8 (8)

atoms	bond angle (°)	atoms	bond angle (°)
Na ^{xiii} —Ca2—O2 ^{xiii}	47.0 (7)	Ca1 ^v —O1—Ca3 ^{vi}	100.1 (9)
Na ^{xiii} —Ca2—O3 ^{xiv}	103.4 (7)	Ca1 ^v —O1—P ⁱ	152.5 (14)
Na ^{xiii} —Ca2—O4 ^v	54.7 (4)	Ca2 ^v —O1—Ca3 ^{vi}	127.2 (10)
Na ^{xiii} —Ca2—O5	104.1 (6)	Ca2 ^v —O1—P ⁱ	92.3 (11)
Na ^{xiii} —Ca2—O6 ^{vi}	123.6 (8)	Ca3 ^{vi} —O1—P ⁱ	96.6 (11)
Na ^{xiii} —Ca2—O7 ^{vi}	129.6 (6)	Na—O2—Na ^{ix}	175.7 (10)
Na ^{xiii} —Ca2—O8 ^{xvii}	53.6 (6)	Na—O2—Ca2 ⁱⁱⁱ	94.4 (8)
Na ^{xiv} —Ca2—Na ^{vi}	103.1 (3)	Na—O2—Ca3 ^{vi}	96.5 (9)
Na ^{xiv} —Ca2—Ca1 ^{xv}	155.0 (3)	Na—O2—P	96.1 (11)
Na ^{xiv} —Ca2—Ca1	77.9 (3)	Na ^{ix} —O2—Ca2 ⁱⁱⁱ	81.3 (9)
Na ^{xiv} —Ca2—Ca1 ^v	63.3 (3)	Na ^{ix} —O2—Ca3 ^{vi}	84.5 (8)
Na ^{xiv} —Ca2—Ca3 ^{xvi}	64.9 (3)	Na ^{ix} —O2—P	85.4 (10)
Na ^{xiv} —Ca2—Ca3 ^{vi}	98.2 (3)	Ca2 ⁱⁱⁱ —O2—Ca3 ^{vi}	97.7 (10)
Na ^{xiv} —Ca2—Si ^{vi}	132.8 (4)	Ca2 ⁱⁱⁱ —O2—P	114.4 (11)
Na ^{xiv} —Ca2—O1 ^{vi}	71.1 (5)	Ca3 ^{vi} —O2—P	144.3 (13)
Na ^{xiv} —Ca2—O2 ^{xiii}	104.2 (6)	Na—O3—Ca2 ^{iv}	93.7 (8)
Na ^{xiv} —Ca2—O3 ^{xiv}	46.5 (7)	Na—O3—Ca3 ^{vii}	99.6 (9)
Na ^{xiv} —Ca2—O4 ^v	40.8 (4)	Na—O3—P	101.9 (13)
Na ^{xiv} —Ca2—O5	47.8 (5)	Ca2 ^{iv} —O3—Ca3 ^{vii}	94.7 (11)
Na ^{xiv} —Ca2—O6 ^{vi}	122.8 (7)	Ca2 ^{iv} —O3—P	108.4 (12)
Na ^{xiv} —Ca2—O7 ^{vi}	122.9 (7)	Ca3 ^{vii} —O3—P	147.1 (14)
Na ^{xiv} —Ca2—O8 ^{xvii}	108.5 (7)	Na ^{ix} —O4—Ca1	99.0 (7)
Na ^{vi} —Ca2—Ca1 ^{xv}	101.9 (3)	Na ^{ix} —O4—Ca2 ^{vi}	92.7 (6)
Na ^{vi} —Ca2—Ca1	102.0 (3)	Na ^{ix} —O4—Ca3 ^{xxii}	99.5 (8)
Na ^{vi} —Ca2—Ca1 ^v	153.5 (3)	Na ^{ix} —O4—P	112.9 (11)
Na ^{vi} —Ca2—Ca3 ^{xvi}	60.3 (3)	Ca1—O4—Ca2 ^{vi}	88.1 (6)
Na ^{vi} —Ca2—Ca3 ^{vi}	148.1 (2)	Ca1—O4—Ca3 ^{xxii}	159.1 (7)
Na ^{vi} —Ca2—Si ^{vi}	72.0 (3)	Ca1—O4—P	89.0 (11)
Na ^{vi} —Ca2—O1 ^{vi}	68.4 (6)	Ca2 ^{vi} —O4—Ca3 ^{xxii}	81.5 (5)
Na ^{vi} —Ca2—O2 ^{xiii}	55.4 (7)	Ca2 ^{vi} —O4—P	154.4 (12)
Na ^{vi} —Ca2—O3 ^{xiv}	56.6 (7)	Ca3 ^{xxii} —O4—P	92.6 (11)
Na ^{vi} —Ca2—O4 ^v	108.0 (5)	Na ^{xiv} —O5—Ca1 ^v	92.5 (6)
Na ^{vi} —Ca2—O5	142.0 (7)	Na ^{xiv} —O5—Ca2	91.3 (7)
Na ^{vi} —Ca2—O6 ^{vi}	106.3 (6)	Na ^{xiv} —O5—Ca3 ^{vi}	174.2 (11)
Na ^{vi} —Ca2—O7 ^{vi}	42.7 (4)	Na ^{xiv} —O5—Si	86.9 (12)
Na ^{vi} —Ca2—O8 ^{xvii}	141.3 (8)	Ca1 ^v —O5—Ca2	94.9 (8)
Ca1 ^{xv} —Ca2—Ca1	96.6 (2)	Ca1 ^v —O5—Ca3 ^{vi}	82.3 (7)
Ca1 ^{xv} —Ca2—Ca1 ^v	93.7 (2)	Ca1 ^v —O5—Si	106.7 (12)
Ca1 ^{xv} —Ca2—Ca3 ^{xvi}	130.2 (4)	Ca2—O5—Ca3 ^{vi}	86.8 (8)
Ca1 ^{xv} —Ca2—Ca3 ^{vi}	59.1 (3)	Ca2—O5—Si	158.4 (14)
Ca1 ^{xv} —Ca2—Si ^{vi}	56.5 (3)	Ca3 ^{vi} —O5—Si	96.9 (10)
Ca1 ^{xv} —Ca2—O1 ^{vi}	118.7 (5)	Na ^{xiv} —O6—Ca1 ^v	94.2 (8)
Ca1 ^{xv} —Ca2—O2 ^{xiii}	90.2 (6)	Na ^{xiv} —O6—Ca1 ^{xviii}	91.4 (8)
Ca1 ^{xv} —Ca2—O3 ^{xiv}	158.5 (7)	Na ^{xiv} —O6—Ca2 ^v	177.5 (12)
Ca1 ^{xv} —Ca2—O4 ^v	129.1 (5)	Na ^{xiv} —O6—Ca3	89.5 (7)

atoms	bond angle (°)	atoms	bond angle (°)
Ca1 ^{xv} —Ca2—O5	109.3 (5)	Na ^{xiv} —O6—Si	89.2 (11)
Ca1 ^{xv} —Ca2—O6 ^{vi}	47.9 (7)	Ca1 ^v —O6—Ca1 ^{xviii}	173.6 (10)
Ca1 ^{xv} —Ca2—O7 ^{vi}	76.7 (6)	Ca1 ^v —O6—Ca2 ^v	88.0 (9)
Ca1 ^{xv} —Ca2—O8 ^{xvii}	49.0 (7)	Ca1 ^v —O6—Ca3	88.3 (9)
Ca1—Ca2—Ca1 ^v	97.3 (2)	Ca1 ^v —O6—Si	93.0 (14)
Ca1—Ca2—Ca3 ^{xvi}	131.2 (4)	Ca1 ^{xviii} —O6—Ca2 ^v	86.5 (8)
Ca1—Ca2—Ca3 ^{vi}	59.6 (3)	Ca1 ^{xviii} —O6—Ca3	88.6 (9)
Ca1—Ca2—Si ^{vi}	58.5 (3)	Ca1 ^{xviii} —O6—Si	90.2 (13)
Ca1—Ca2—O1 ^{vi}	37.5 (5)	Ca2 ^v —O6—Ca3	91.9 (9)
Ca1—Ca2—O2 ^{xiii}	157.4 (7)	Ca2 ^v —O6—Si	89.3 (9)
Ca1—Ca2—O3 ^{xiv}	89.1 (7)	Ca3—O6—Si	178.2 (17)
Ca1—Ca2—O4 ^v	115.6 (4)	Na—O7—Ca2 ^v	88.8 (7)
Ca1—Ca2—O5	54.1 (5)	Na—O7—Ca3 ^{vi}	94.6 (9)
Ca1—Ca2—O6 ^{vi}	48.8 (7)	Na—O7—Si	167.0 (16)
Ca1—Ca2—O7 ^{vi}	71.4 (5)	Ca2 ^v —O7—Ca3 ^{vi}	121.0 (9)
Ca1—Ca2—O8 ^{xvii}	105.8 (7)	Ca2 ^v —O7—Si	96.0 (10)
Ca1 ^v —Ca2—Ca3 ^{xvi}	93.23 (13)	Ca3 ^{vi} —O7—Si	93.3 (12)
Ca1 ^v —Ca2—Ca3 ^{vi}	58.38 (18)	Ca1 ^{xxiii} —O8—Ca1 ^v	169.3 (10)
Ca1 ^v —Ca2—Si ^{vi}	134.3 (3)	Ca1 ^{xxiii} —O8—Ca2 ^{xxiv}	93.8 (10)
Ca1 ^v —Ca2—O1 ^{vi}	121.9 (6)	Ca1 ^{xxiii} —O8—Ca3 ^{xv}	85.8 (9)
Ca1 ^v —Ca2—O2 ^{xiii}	103.8 (7)	Ca1 ^{xxiii} —O8—Si ^v	96.2 (12)
Ca1 ^v —Ca2—O3 ^{xiv}	106.1 (7)	Ca1 ^v —O8—Ca2 ^{xxiv}	87.8 (8)
Ca1 ^v —Ca2—O4 ^v	46.4 (5)	Ca1 ^v —O8—Ca3 ^{xv}	83.7 (7)
Ca1 ^v —Ca2—O5	45.2 (5)	Ca1 ^v —O8—Si ^v	86.0 (13)
Ca1 ^v —Ca2—O6 ^{vi}	100.1 (6)	Ca2 ^{xxiv} —O8—Ca3 ^{xv}	89.8 (10)
Ca1 ^v —Ca2—O7 ^{vi}	163.8 (5)	Ca2 ^{xxiv} —O8—Si ^v	157.4 (17)
Ca1 ^v —Ca2—O8 ^{xvii}	45.3 (7)	Ca3 ^{xv} —O8—Si ^v	111.0 (13)
Ca3 ^{xvi} —Ca2—Ca3 ^{vi}	151.60 (17)		

symmetry codes: (i) $-x+3/2, y-1/2, z+1/2$; (ii) $-x+3/2, y+1/2, z+1/2$; (iii) $x+1/2, -y+1/2, z$;
 (iv) $x+1/2, -y+3/2, z$; (v) $-x+1, -y+1, z+1/2$; (vi) $-x+1, -y+1, z-1/2$; (vii) $-x+1, -y+2, z-1/2$;
 (viii) $-x+3/2, y+1/2, z-1/2$; (ix) $-x+3/2, y-1/2, z-1/2$; (x) $x, y+1, z$; (xi) $x, y, z-1$;
 (xii) $x, y+1, z-1$; (xiii) $x-1/2, -y+1/2, z$; (xiv) $x-1/2, -y+3/2, z$; (xv) $x, y-1, z$;
 (xvi) $-x+1/2, y-1/2, z-1/2$; (xvii) $-x+1, -y, z-1/2$; (xviii) $-x+1, -y+2, z+1/2$; (xix) $x, y, z+1$;
 (xx) $-x+1/2, y+1/2, z+1/2$; (xxi) $x-1/2, -y+3/2, z+1$; (xxii) $x+1/2, -y+3/2, z-1$;
 (xxiii) $x, y-1, z+1$; (xxiv) $-x+1, -y, z+1/2$.

Table S3 Luminescence decay parameters of NaCa₃PSiO₈:Eu²⁺ phosphor based on three components exponential decay model.

compound	decay parameters					
	I_1	τ_1 (μ s)	I_2	τ_2 (μ s)	I_3	τ_3 (μ s)
NaCa ₃ PSiO ₈ :0.0125Eu ²⁺	0.70	0.15	0.18	0.30	0.12	0.76
NaCa ₃ PSiO ₈ :0.025Eu ²⁺	0.76	0.106	0.14	0.21	0.10	0.53

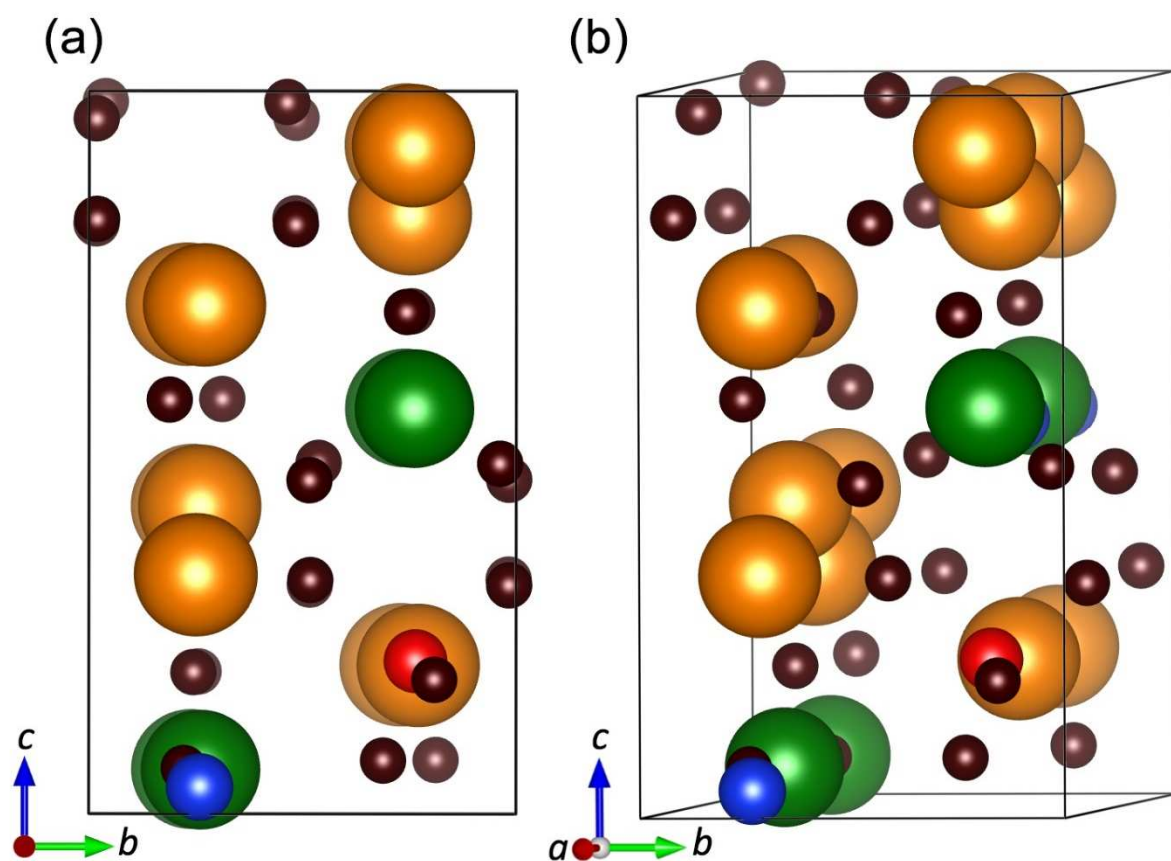


Figure S1 (a) Unit cell of $\text{NaCa}_3\text{PSiO}_8$ along the (100) plane depicting cation channel along the a axis of the unit cell, (b) the view along a slightly inclined angle.

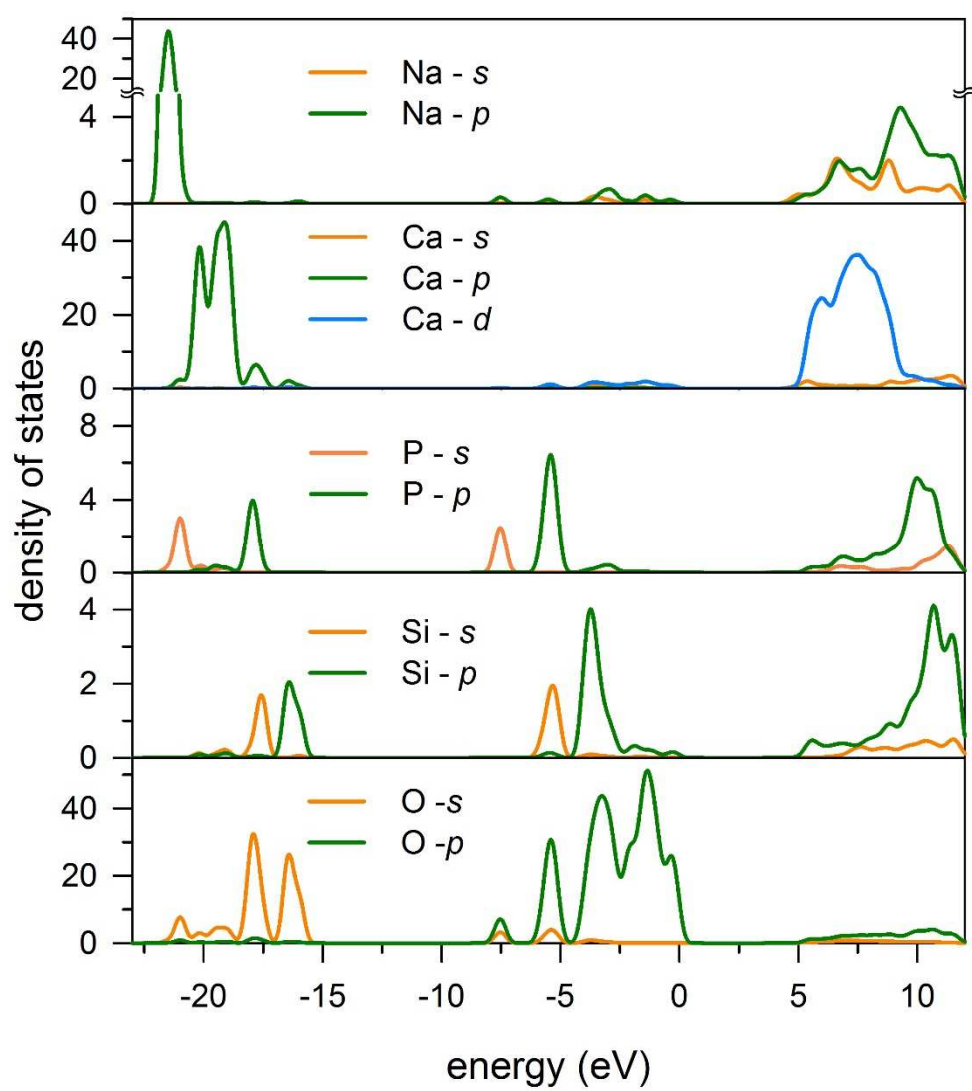


Figure S2 The partial density of states of the atoms in the electronic structure of NaCa₃PSiO₈.