Supporting Information

$Ba_3[Al(PO_4)_3]$: Rational Design of a Promising Deep-UV Transparent SHG Crystal with Balanced Overall Performance Originated from the Condensation of Quartz-Type $[Al(PO_4)_4]^{9-}$ Units

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Experimental Procedures

Crystal Growth of BAPO

Single crystals of BAPO were obtained by a spontaneous nucleation method. Raw materials of $BaCO_3$ (99.9%, Aladdin Co.), Al_2O_3 (99.9%, Aladdin Co.) and $NH_4H_2PO_4$ (99.9%, Aladdin Co.) in a molar ratio of 3:1:3 were ground and blended into a φ40 platinum crucible, and followed by 7 days' holding at 1323.15 K with a crystal growing furnace. After a slow cooling to 1073.15K within one month and a rapid cooling to room temperature within one day, rod-like colorless crystals of BAPO were observed at the surface.

Single Crystal and Powder X-ray Diffraction

A colorless rod-like crystal with dimensions of 0.17×0.10×0.05mm^3 was selected for single-crystal X-ray diffraction. The diffraction data were collected on an Agilent Technologies Super Nova Dual Wavelength CCD diffractometer equipped with graphite-monochromatic Mo Kα radiation (λ= 0.71073 Å) at 100 K and data reduction was done by using CrysAlisPro software. The crystal structure was solved by the direct methods and refined by full matrix least squares on F^2 by SHELXL-2017 program [1]. The structure was verified using the ADDSYM algorithm from the program PLATON [2], and no higher symmetry was found. The diffraction data of powder samples was collected by powder X-ray diffraction measurement on a Rigaku Mini Flex II X-ray diffractometer using Cu Kα radiation (λ= 1.5418Å) at room temperature in the angular range of 2θ = 10-70° with a scan step width of 0.02° and a scan rate of 2.5°/min, while in situ powder X-ray diffraction measurements in the angular range of 2θ = 10-70° with a scan step width of 0.02° and a scan rate of 2.5°/min were performed on a Rigaku ULTIMA IV X-ray diffractometer using Cu Kα radiation (λ= 1.5418Å) at variable temperatures of 450°C, 500°C, 550°C in the heating process and 300°C in the cooling process.

UV-Vis-NIR diffuse reflectance spectrum

The reflection spectrum of BAPO crystal was performed with a PE Lambda 950 UV-vis-NIR spectrophotometer in the range of 200–1100 nm, while the reflectance of $BaSO_4$ plate was used as the referential standard (100 % reflectance).

Thermal Analysis

Thermogravimetric analyses (TGA) and differential scanning calorimetry (DSC) measurements were performed on a NETZSCH STA 449C apparatus using Al_2O_3 as reference material under N_2 flow with a sample heating rate of

20.0k/min from 50℃ to 1100℃. After the measurement, the sample was checked by powder XRD.

Powder Second Harmonic Generation Measurement

SHG Measurements for BAPO were carried out with a Nd:YAG 1064 nm laser. Sieved KDP sample with particle size of 212-270 μm was taken as reference for assuming SHG signals. The samples were ground and sieved into six discrete ranges of particle sizes, namely 45-53, 53-75, 75-109, 109-150, 150-212 and 212-270 μm.

Computational Methods

The calculations of electronic and optical properties were performed with the CASTEP code using the plane-wave pseudopotential density functional theory (DFT) [3]. The generalized gradient approximation (GGA) Perdew-Burke-Ernzerhof (PBE) was chosen as the exchange-correlation functional [4]. The core-electron interactions were represented by the norm-conserving pseudopotential [5]. Al $3s^2$ $3p^1$, O-$2s^2$ $2p^4$, P-$3s^2$ $3p^3$ and Ba-$5s^2$ $5p^6$ $6s^2$ orbital electrons were set as the valence electrons. A cutoff energy of 750 eV was utilized for determination of the number of plane-wave basis sets. Monkhorst-Pack k-point sampling was 2 × 2 × 2 for numerical integration over Brillouin zone. More than 960 empty bands were used during the optical property calculations.

The second-order NLO properties of the material were calculated implementing the length-gauge formalism in the independent-particle approximation. According to the latest research [6], the static SHG susceptibility can be written as $\chi^{\alpha\beta\gamma}$ = $\chi^{\alpha\beta\gamma}$ (VE) + $\chi^{\alpha\beta\gamma}$ (VH), where $\chi^{\alpha\beta\gamma}$ (VE) is contributed by virtual-electron processes and $\chi^{\alpha\beta\gamma}$ (VH) is contributed by virtual-hole processes. The formulas of $\chi^{\alpha\beta\gamma}$(VE) and $\chi^{\alpha\beta\gamma}$(VH) are given in Chen's paper [7].

Energy Dispersive Spectrum

Microprobe elemental analyses for the Ba, Al, Fe and P elements were performed on a field-emission scanning electron microscope (FESEM, JSM6700F) equipped with an energy-dispersive X-ray spectroscope (EDS, Oxford INCA).

Figure S1. PXRD patterns for $Ba_3[Al(PO_4)_3]$.

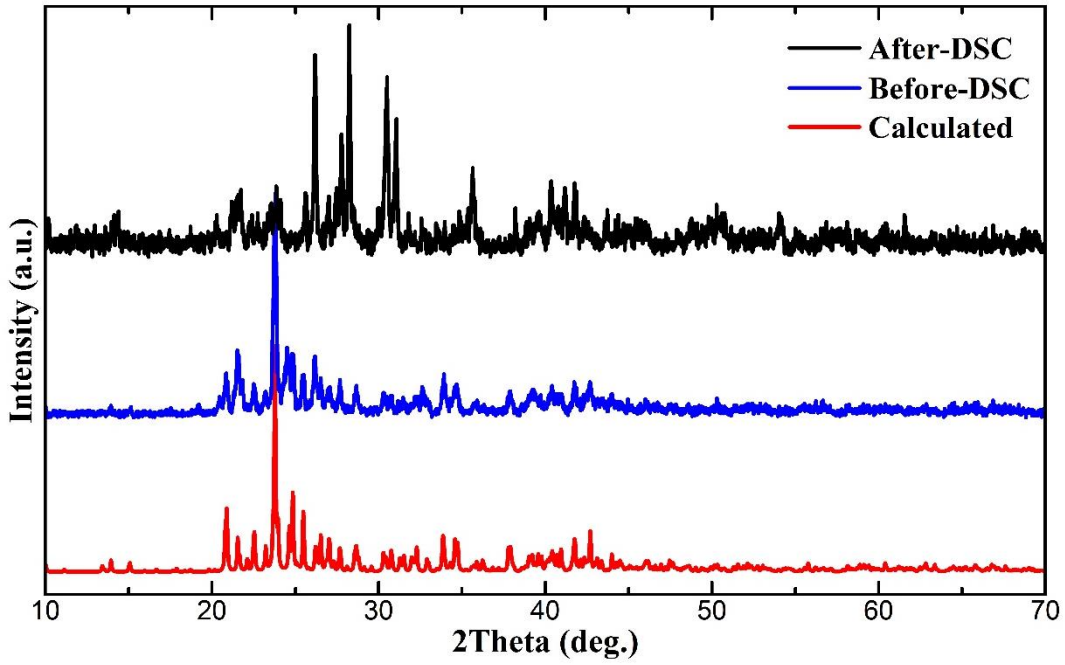


Figure S2. In situ PXRD patterns at varied temperatures for $Ba_3[Al(PO_4)_3]$.

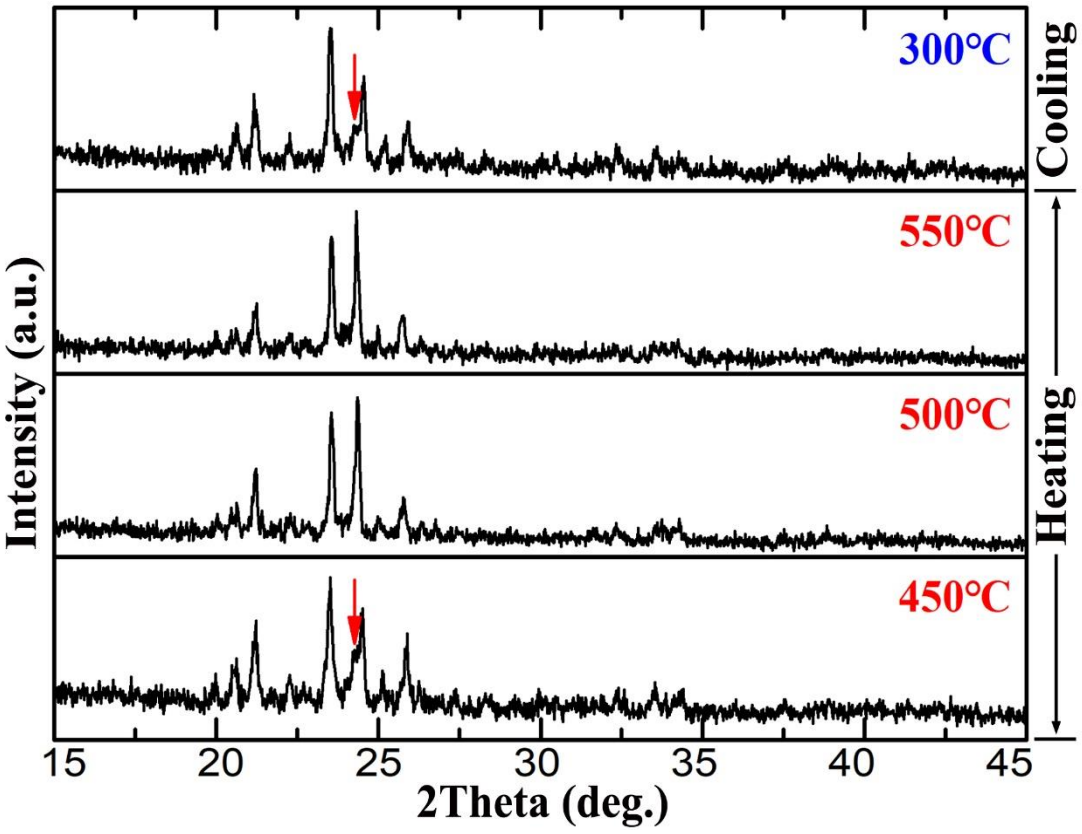


Figure S3. Recorded DSC and TG curves for $Ba_3[Al(PO_4)_3]$.

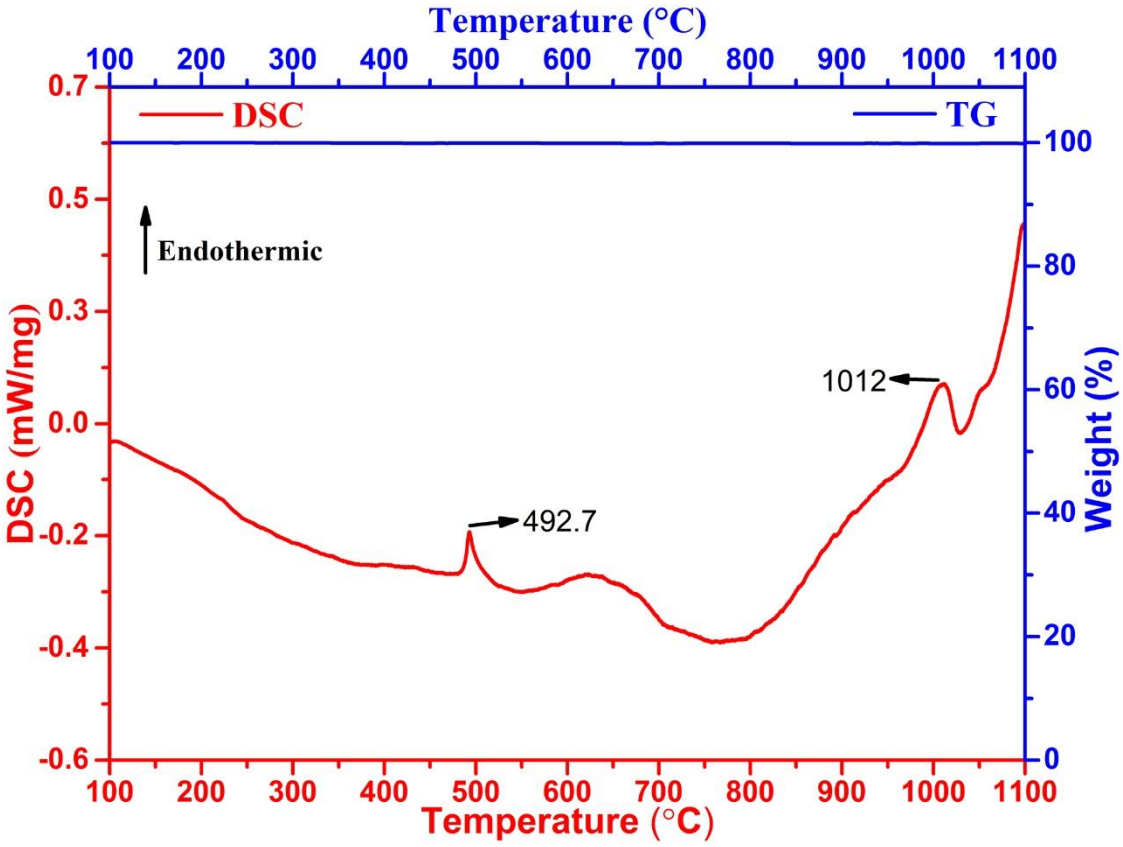
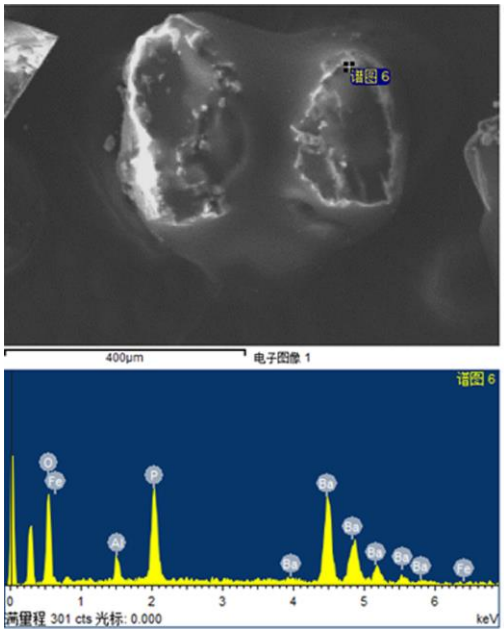


Figure S4. Energy Dispersive Spectrum for $Ba_3[Al(PO_4)_3]$.



element	Weight percentage (%)	Atomic percentage (%)
O K	27.89	63.22
Al K	3.92	5.27
P K	14.87	17.41
Fe K	0.04	0.02
Ba L	53.28	14.07
Total	100.00	

Table S1. Crystal data and structure refinement for $Ba_3[Al(PO_4)_3]$.

Empirical formula	$Ba_3AlP_3O_{12}$
Formula weight	723.91
Temperature/K	100.0(2)
Crystal system	triclinic
Space group	*P*1
a/Å	12.7192(3)
b/Å	12.7916(3)
c/Å	15.8220(4)
α/°	90.058(2)
β/°	90.033(2)
γ/°	111.917(2)
Volume/Å^3	2388.17(10)
Z	8
ρ_{calc}g/cm^3	4.027
μ/mm^{-1}	10.317
F(000)	2576.0
Crystal size/mm^3	0.169 × 0.098 × 0.045
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.854 to 74.312
Index ranges	-21 ≤ h ≤ 21, -21 ≤ k ≤ 21, -26 ≤ l ≤ 26
Reflections collected	78838
Independent reflections	45647 [R_{int} = 0.0390, R_{sigma} = 0.0682]
Data/restraints/parameters	45647/921/1370
Goodness-of-fit on F^2	1.095
Final R indexes [I>=2σ (I)]	R_1 = 0.0451, wR_2 = 0.0852
Final R indexes [all data]	R_1 = 0.0496, wR_2 = 0.0874
Largest diff. peak/hole/eÅ^{-3}	2.47/-2.66
Flack parameter	0.333(12)

Table S2. Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for $Ba_3[Al(PO_4)_3]$.

Atom	*x*	*y*	*z*	U(eq)
Ba01	−0.51233 (5)	0.11937 (5)	0.22968 (4)	0.00546 (9)
Ba02	1.09002 (5)	1.30078 (5)	0.60219 (4)	0.00640 (9)
Ba03	0.16600 (5)	0.34710 (5)	0.18047 (4)	0.00568 (9)
Ba04	−0.15498 (5)	0.22846 (5)	0.38593 (4)	0.00637 (9)
Ba05	1.15953 (5)	1.25100 (5)	0.89616 (4)	0.00674 (10)
Ba06	0.02788 (5)	−0.03437 (5)	0.44091 (4)	0.00594 (9)
Ba07	0.31361 (5)	−0.34116 (5)	0.67515 (4)	0.00533 (9)
Ba08	0.98208 (5)	−0.10854 (5)	0.72554 (4)	0.00638 (10)
Ba11	1.46722 (5)	1.39360 (5)	0.73426 (4)	0.00651 (10)
Ba12	−0.32106 (5)	−0.12406 (5)	0.28675 (4)	0.00544 (9)
Ba13	0.59763 (5)	0.42511 (5)	0.42566 (4)	0.00534 (9)
Ba14	0.87431 (5)	0.58059 (5)	−0.07555 (4)	0.00559 (9)
Ba15	0.79068 (5)	0.14441 (5)	0.79192 (4)	0.00527 (9)
Ba16	0.09114 (5)	−0.10676 (5)	0.00666 (4)	0.00662 (10)
Ba17	1.45280 (5)	1.05758 (5)	0.93946 (4)	0.00559 (9)
Ba18	0.66900 (5)	0.75723 (5)	0.55474 (4)	0.00685 (10)
Ba19	0.94760 (5)	0.60415 (5)	0.53533 (4)	0.00616 (9)
Ba20	1.51243 (5)	0.41130 (5)	1.04001 (4)	0.00742 (10)
Ba21	0.37211 (5)	−0.28288 (5)	0.09503 (4)	0.00706 (10)
Ba22	0.37180 (5)	0.10725 (5)	0.50256 (4)	0.00618 (9)
Ba23	0.30297 (5)	−0.25250 (5)	0.39458 (4)	0.00752 (10)
Ba24	0.60990 (5)	0.77634 (5)	0.87323 (4)	0.00745 (10)
Ba25	0.81637 (6)	0.25546 (5)	0.06630 (4)	0.00990 (11)
Ba26	−0.00363 (5)	−0.39364 (6)	0.23638 (4)	0.00929 (11)
P01	−0.0811 (2)	0.0198 (2)	−0.08902 (17)	0.0053 (4)
P02	−0.4054 (2)	−0.0182 (2)	0.08742 (17)	0.0050 (4)
P03	0.0794 (2)	0.4679 (2)	0.40615 (18)	0.0065 (4)
P04	0.8743 (2)	0.0374 (2)	0.58305 (17)	0.0052 (4)
P05	0.7228 (2)	0.3578 (2)	0.24321 (18)	0.0075 (5)
P06	0.2808 (2)	0.1643 (2)	0.05055 (17)	0.0048 (4)
P07	−0.0533 (2)	0.0560 (2)	0.22969 (18)	0.0071 (5)
P08	0.7396 (2)	0.6842 (2)	0.05415 (18)	0.0076 (5)
P09	0.8192 (2)	0.7245 (2)	0.38207 (18)	0.0070 (4)
P10	0.2946 (2)	0.2249 (2)	0.34194 (17)	0.0063 (4)
P11	0.6698 (2)	0.3105 (2)	0.90351 (18)	0.0073 (5)
P12	1.1881 (2)	0.8412 (2)	0.55174 (17)	0.0045 (4)

P13	0.5201 (2)	−0.0368 (2)	0.74096 (17)	0.0058 (4)
P14	0.6883 (2)	0.3033 (2)	0.57120 (18)	0.0071 (4)
P15	1.2412 (2)	1.1587 (2)	0.67904 (17)	0.0062 (4)
P16	0.5411 (2)	−0.0249 (2)	0.41470 (18)	0.0059 (4)
P17	0.7529 (2)	0.6593 (2)	0.72813 (18)	0.0064 (4)
P18	1.3747 (2)	0.5270 (2)	0.88519 (18)	0.0071 (4)
P19	0.4281 (2)	0.5174 (2)	0.55569 (17)	0.0069 (4)
P20	0.4561 (2)	0.5708 (2)	0.24192 (18)	0.0075 (4)
P21	1.1879 (2)	0.7898 (2)	0.84721 (17)	0.0064 (4)
P22	1.0031 (2)	0.4538 (2)	0.73871 (18)	0.0065 (4)
A01	0.7637 (3)	0.4304 (3)	0.7331 (2)	0.0058 (5)
A02	1.1561 (3)	0.5603 (3)	0.8853 (2)	0.0060 (5)
A03	1.2841 (3)	0.9620 (3)	0.7147 (2)	0.0060 (5)
P23	0.2168 (2)	−0.1508 (2)	0.18452 (17)	0.0069 (4)
A04	0.6512 (3)	0.0667 (3)	0.5794 (2)	0.0052 (5)
P24	1.0648 (2)	0.4968 (2)	1.05951 (18)	0.0076 (5)
A05	0.3091 (3)	0.4569 (3)	0.3922 (2)	0.0058 (5)
A06	0.1822 (3)	0.0518 (3)	0.2144 (2)	0.0064 (5)
A07	0.6891 (3)	0.5803 (3)	0.2354 (2)	0.0061 (5)
A08	−0.1911 (3)	−0.0697 (3)	0.0802 (2)	0.0050 (5)
O01	0.3985 (6)	0.1788 (7)	0.0826 (5)	0.0077 (12)
O02	0.2155 (6)	0.1386 (7)	0.3998 (5)	0.0097 (13)
O03	1.0697 (6)	0.8286 (7)	0.5838 (5)	0.0074 (12)
O04	0.0724 (7)	0.5832 (7)	0.3914 (5)	0.0103 (13)
O05	0.5425 (7)	0.5151 (7)	0.5808 (5)	0.0094 (13)
O06	0.8032 (6)	0.8317 (7)	0.4099 (5)	0.0085 (13)
O07	−0.4174 (6)	0.0959 (6)	0.0808 (5)	0.0064 (12)
O08	−0.0696 (7)	0.1423 (6)	−0.0801 (5)	0.0079 (13)
O09	0.7073 (7)	0.3873 (7)	0.9813 (5)	0.0104 (14)
O10	0.3358 (7)	0.4612 (7)	0.6208 (5)	0.0103 (14)
O11	1.2058 (6)	1.0464 (6)	0.7328 (5)	0.0080 (12)
O12	0.6862 (7)	0.2002 (7)	0.9190 (5)	0.0099 (13)
O13	0.6858 (7)	0.3204 (7)	0.6691 (5)	0.0121 (14)
O14	−0.0002 (7)	0.4048 (7)	0.4786 (5)	0.0123 (14)
O15	1.2089 (6)	0.8937 (6)	0.4637 (5)	0.0076 (12)
O16	0.1846 (6)	0.0765 (6)	0.1063 (5)	0.0074 (12)
O17	0.3991 (7)	0.4484 (8)	0.4703 (6)	0.0135 (15)
O18	0.9424 (7)	0.7364 (7)	0.3794 (5)	0.0107 (13)
O19	1.2052 (6)	0.7289 (6)	0.5525 (5)	0.0076 (12)
O20	0.6019 (6)	0.0574 (6)	0.6827 (5)	0.0070 (12)

O21	−0.1288 (7)	−0.0519 (6)	0.1799 (5)	0.0089 (13)
O22	0.9074 (7)	0.0953 (6)	0.6684 (5)	0.0089 (13)
O23	0.2528 (7)	−0.0372 (7)	0.2383 (5)	0.0113 (14)
O24	0.2417 (7)	−0.2391 (7)	0.2365 (5)	0.0104 (13)
O25	0.4363 (6)	−0.0150 (7)	0.3745 (5)	0.0083 (13)
O26	0.9476 (7)	0.5017 (7)	1.0704 (5)	0.0112 (14)
O27	−0.2737 (7)	0.0122 (7)	0.0792 (5)	0.0094 (13)
O28	0.8986 (6)	−0.0714 (6)	0.5802 (5)	0.0070 (12)
O29	1.4275 (7)	0.5868 (7)	0.8026 (5)	0.0091 (13)
O30	−0.1843 (7)	−0.0464 (7)	−0.1415 (5)	0.0090 (13)
O31	0.6698 (7)	0.2932 (7)	0.3232 (5)	0.0093 (13)
O32	0.9071 (7)	0.4954 (7)	0.7091 (5)	0.0102 (13)
O33	−0.1185 (7)	0.0604 (7)	0.3089 (5)	0.0126 (15)
O34	−0.4661 (6)	−0.0991 (7)	0.0153 (5)	0.0086 (13)
O35	0.2635 (7)	0.3323 (7)	0.3375 (5)	0.0091 (13)
O36	0.0566 (7)	0.3977 (8)	0.3257 (6)	0.0139 (15)
O37	0.6974 (7)	0.5260 (7)	0.7418 (6)	0.0108 (14)
O38	0.6598 (7)	0.7056 (7)	0.7232 (5)	0.0105 (13)
O39	0.3909 (7)	0.5004 (7)	0.1683 (6)	0.0131 (15)
O40	0.0276 (6)	0.0138 (7)	−0.1249 (5)	0.0073 (12)
O41	0.9320 (6)	0.1171 (6)	0.5108 (5)	0.0069 (12)
O42	1.4119 (7)	0.6064 (7)	0.9594 (6)	0.0116 (14)
O43	0.2645 (6)	0.2772 (6)	0.0526 (5)	0.0071 (12)
O44	0.0511 (7)	0.0281 (7)	0.2596 (5)	0.0103 (13)
O45	1.2839 (6)	0.9283 (6)	0.6082 (5)	0.0067 (12)
O46	0.4824 (8)	−0.1508 (7)	0.6994 (6)	0.0149 (15)
O47	0.5494 (7)	0.2921 (7)	0.8755 (6)	0.0134 (15)
O48	0.5400 (7)	0.0133 (7)	0.5095 (5)	0.0092 (13)
O49	1.1035 (7)	0.5088 (7)	0.6821 (5)	0.0107 (14)
O50	1.3971 (7)	0.4185 (7)	0.8959 (5)	0.0085 (13)
O51	0.7656 (7)	0.4094 (7)	0.5276 (6)	0.0122 (14)
O52	0.7513 (7)	0.6295 (7)	0.4409 (5)	0.0126 (14)
O53	0.6495 (6)	0.0488 (6)	0.3707 (5)	0.0099 (13)
O54	0.5314 (7)	−0.1483 (7)	0.4153 (5)	0.0101 (13)
O55	0.8295 (7)	0.7090 (7)	0.8037 (5)	0.0129 (15)
O56	−0.4470 (8)	−0.0707 (7)	0.1731 (5)	0.0133 (15)
O57	0.2768 (7)	0.1842 (7)	0.2484 (5)	0.0097 (13)
O58	0.4358 (7)	0.6373 (7)	0.5367 (5)	0.0103 (14)
O59	1.0652 (7)	0.7471 (6)	0.8760 (5)	0.0102 (14)
O60	1.3675 (7)	1.1918 (7)	0.6611 (5)	0.0117 (14)

O61	0.8202 (7)	0.6827 (7)	0.6458 (5)	0.0097 (13)
O62	0.7357 (7)	0.2087 (7)	0.5587 (5)	0.0087 (13)
O63	0.5706 (7)	0.2649 (7)	0.5365 (5)	0.0100 (13)
O64	0.5797 (7)	−0.0292 (7)	0.8248 (5)	0.0092 (13)
O65	0.2590 (7)	0.1120 (7)	−0.0379 (5)	0.0077 (12)
O66	1.0265 (7)	0.4942 (7)	0.8319 (5)	0.0117 (14)
O67	0.7119 (7)	0.7913 (6)	0.0726 (6)	0.0100 (13)
O68	0.9610 (7)	0.3260 (6)	0.7351 (5)	0.0095 (13)
O69	1.2198 (7)	1.2483 (6)	0.7331 (5)	0.0079 (13)
O70	0.4183 (7)	0.2522 (7)	0.3644 (5)	0.0104 (13)
O71	1.1934 (7)	0.8322 (6)	0.7551 (5)	0.0095 (13)
O72	0.7546 (7)	0.4885 (7)	0.2651 (5)	0.0098 (13)
O73	0.7411 (7)	−0.0050 (6)	0.5706 (5)	0.0088 (13)
O74	−0.0198 (7)	0.1582 (7)	0.1743 (6)	0.0123 (14)
O75	1.2394 (7)	0.4825 (7)	0.8737 (5)	0.0103 (13)
O76	0.2046 (7)	0.4919 (8)	0.4384 (6)	0.0144 (15)
O77	0.6781 (7)	0.6272 (7)	−0.0260 (5)	0.0113 (14)
O78	−0.0915 (7)	−0.0344 (7)	0.0014 (5)	0.0101 (13)
O79	0.4191 (6)	0.0009 (6)	0.7583 (5)	0.0075 (12)
O80	1.2641 (7)	0.8808 (6)	0.9040 (5)	0.0102 (13)
O81	0.0902 (7)	−0.1862 (7)	0.1681 (5)	0.0118 (14)
O82	1.1375 (7)	0.5380 (7)	1.1392 (5)	0.0097 (13)
O83	0.5117 (7)	0.6940 (7)	0.2206 (6)	0.0132 (15)
O84	1.2321 (7)	0.6896 (6)	0.8393 (5)	0.0096 (13)
O85	1.0554 (7)	0.3778 (7)	1.0346 (6)	0.0124 (14)
O86	0.2824 (7)	−0.1250 (7)	0.1018 (5)	0.0121 (14)
O87	0.8678 (7)	0.7160 (7)	0.0502 (6)	0.0122 (14)
O88	0.7678 (7)	0.7014 (7)	0.2884 (5)	0.0116 (14)
O89	0.7596 (7)	0.3725 (7)	0.8317 (5)	0.0100 (13)
O90	1.1728 (7)	1.1343 (7)	0.5979 (5)	0.0116 (14)
O91	0.8330 (7)	0.3433 (8)	0.2255 (6)	0.0148 (15)
O92	0.3746 (8)	0.5621 (7)	0.3182 (6)	0.0144 (15)
O93	0.6843 (7)	0.6001 (7)	0.1273 (5)	0.0096 (13)
O94	1.1272 (8)	0.5836 (7)	0.9885 (5)	0.0147 (15)
O95	0.5482 (7)	0.5266 (7)	0.2737 (5)	0.0101 (13)
O96	0.6397 (8)	0.3272 (7)	0.1694 (6)	0.0157 (16)

Table S3. Anisotropic Displacement Parameters (Å^2) for $Ba_3[Al(PO_4)_3]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ba01	0.0047 (2)	0.0062 (2)	0.0056 (2)	0.00208 (18)	0.00068 (17)	0.00069 (17)
Ba02	0.0067 (2)	0.0057 (2)	0.0068 (2)	0.00239 (19)	−0.00116 (18)	0.00007 (17)
Ba03	0.0061 (2)	0.0054 (2)	0.0052 (2)	0.00165 (18)	0.00017 (18)	0.00004 (17)
Ba04	0.0057 (2)	0.0048 (2)	0.0086 (2)	0.00188 (18)	−0.00140 (18)	−0.00035 (18)
Ba05	0.0052 (2)	0.0069 (2)	0.0072 (2)	0.00116 (19)	−0.00126 (18)	0.00174 (18)
Ba06	0.0049 (2)	0.0065 (2)	0.0068 (2)	0.00243 (18)	0.00117 (18)	0.00077 (18)
Ba07	0.0048 (2)	0.0047 (2)	0.0053 (2)	0.00040 (18)	−0.00029 (17)	−0.00023 (17)
Ba08	0.0044 (2)	0.0078 (2)	0.0057 (2)	0.00081 (19)	−0.00053 (18)	−0.00088 (18)
Ba11	0.0044 (2)	0.0076 (2)	0.0072 (2)	0.00183 (19)	0.00021 (18)	0.00105 (18)
Ba12	0.0043 (2)	0.0060 (2)	0.0062 (2)	0.00201 (18)	−0.00025 (17)	−0.00034 (17)
Ba13	0.0047 (2)	0.0046 (2)	0.0064 (2)	0.00130 (18)	−0.00019 (17)	−0.00003 (17)
Ba14	0.0052 (2)	0.0043 (2)	0.0067 (2)	0.00109 (18)	0.00039 (18)	0.00021 (17)
Ba15	0.0038 (2)	0.0058 (2)	0.0060 (2)	0.00156 (18)	0.00013 (17)	−0.00014 (17)
Ba16	0.0065 (2)	0.0072 (2)	0.0067 (2)	0.00327 (19)	−0.00192 (18)	−0.00198 (18)
Ba17	0.0053 (2)	0.0061 (2)	0.0062 (2)	0.00302 (18)	−0.00095 (18)	−0.00089 (17)
Ba18	0.0071 (2)	0.0048 (2)	0.0075 (2)	0.00085 (19)	−0.00084 (18)	0.00001 (18)
Ba19	0.0049 (2)	0.0046 (2)	0.0074 (2)	−0.00001 (18)	0.00136 (18)	−0.00013 (18)
Ba20	0.0056 (2)	0.0060 (2)	0.0089 (2)	0.00011 (19)	−0.00061 (19)	−0.00089 (18)
Ba21	0.0080 (2)	0.0059 (2)	0.0075 (2)	0.00274 (19)	0.00147 (19)	0.00013 (18)
Ba22	0.0055 (2)	0.0066 (2)	0.0060 (2)	0.00191 (18)	−0.00005 (18)	0.00117 (18)
Ba23	0.0064 (2)	0.0082 (2)	0.0069 (2)	0.00138 (19)	0.00097 (19)	−0.00151 (19)
Ba24	0.0073 (2)	0.0053 (2)	0.0092 (2)	0.00181 (19)	0.00163 (19)	0.00086 (18)
Ba25	0.0110 (3)	0.0063 (2)	0.0089 (3)	−0.0008 (2)	−0.0014 (2)	0.00192 (19)
Ba26	0.0065 (2)	0.0122 (3)	0.0081 (2)	0.0023 (2)	0.00096 (19)	−0.0011 (2)
P01	0.0047 (10)	0.0067 (10)	0.0048 (10)	0.0027 (8)	−0.0002 (8)	0.0011 (8)
P02	0.0038 (10)	0.0042 (10)	0.0069 (10)	0.0013 (8)	0.0003 (8)	0.0010 (8)
P03	0.0058 (10)	0.0061 (10)	0.0089 (11)	0.0035 (9)	−0.0030 (9)	−0.0027 (8)
P04	0.0037 (10)	0.0051 (10)	0.0060 (10)	0.0007 (8)	−0.0001 (8)	0.0002 (8)
P05	0.0079 (11)	0.0055 (10)	0.0093 (11)	0.0028 (9)	0.0020 (9)	0.0004 (9)
P06	0.0036 (10)	0.0047 (10)	0.0061 (10)	0.0017 (8)	−0.0001 (8)	0.0002 (8)
P07	0.0045 (10)	0.0057 (10)	0.0089 (11)	−0.0008 (8)	0.0022 (9)	−0.0010 (8)
P08	0.0090 (11)	0.0056 (10)	0.0081 (11)	0.0026 (9)	0.0015 (9)	0.0008 (8)
P09	0.0067 (11)	0.0080 (11)	0.0070 (11)	0.0033 (9)	−0.0027 (9)	−0.0034 (8)
P10	0.0066 (10)	0.0048 (10)	0.0074 (11)	0.0022 (8)	−0.0009 (9)	−0.0004 (8)
P11	0.0056 (10)	0.0071 (11)	0.0096 (11)	0.0028 (9)	0.0030 (9)	0.0020 (9)
P12	0.0032 (10)	0.0048 (10)	0.0047 (10)	0.0006 (8)	0.0004 (8)	0.0000 (8)
P13	0.0039 (10)	0.0043 (10)	0.0079 (11)	0.0001 (8)	−0.0024 (8)	0.0004 (8)

P14	0.0058 (10)	0.0059 (10)	0.0087 (11)	0.0011 (9)	−0.0021 (9)	−0.0012 (8)
P15	0.0074 (11)	0.0063 (10)	0.0064 (10)	0.0045 (9)	0.0003 (8)	−0.0001 (8)
P16	0.0044 (10)	0.0056 (10)	0.0075 (11)	0.0017 (8)	0.0003 (8)	−0.0014 (8)
P17	0.0063 (11)	0.0038 (10)	0.0092 (11)	0.0018 (8)	0.0003 (9)	−0.0003 (8)
P18	0.0046 (10)	0.0081 (11)	0.0090 (11)	0.0028 (9)	0.0016 (9)	0.0015 (9)
P19	0.0093 (11)	0.0061 (10)	0.0050 (10)	0.0024 (9)	−0.0009 (9)	−0.0009 (8)
P20	0.0068 (11)	0.0078 (11)	0.0065 (11)	0.0011 (9)	−0.0013 (9)	0.0009 (8)
P21	0.0060 (10)	0.0056 (10)	0.0076 (11)	0.0021 (8)	0.0022 (8)	0.0006 (8)
P22	0.0052 (10)	0.0067 (10)	0.0060 (10)	0.0004 (8)	0.0013 (8)	−0.0010 (8)
A01	0.0060 (13)	0.0039 (12)	0.0067 (13)	0.0008 (10)	−0.0002 (10)	0.0013 (10)
A02	0.0054 (13)	0.0049 (13)	0.0077 (13)	0.0021 (10)	0.0005 (10)	0.0003 (10)
A03	0.0043 (12)	0.0070 (13)	0.0065 (13)	0.0019 (10)	−0.0017 (10)	−0.0009 (10)
P23	0.0072 (11)	0.0070 (10)	0.0070 (11)	0.0034 (9)	−0.0013 (9)	−0.0005 (8)
A04	0.0058 (13)	0.0048 (12)	0.0054 (12)	0.0024 (10)	−0.0005 (10)	0.0005 (10)
P24	0.0103 (11)	0.0057 (10)	0.0058 (11)	0.0019 (9)	0.0000 (9)	0.0011 (8)
A05	0.0055 (13)	0.0074 (13)	0.0055 (13)	0.0035 (11)	−0.0007 (10)	−0.0004 (10)
A06	0.0060 (13)	0.0058 (13)	0.0071 (13)	0.0020 (11)	0.0008 (10)	0.0004 (10)
A07	0.0076 (13)	0.0054 (13)	0.0053 (13)	0.0024 (11)	−0.0014 (10)	0.0001 (10)
A08	0.0048 (13)	0.0065 (13)	0.0041 (12)	0.0028 (10)	−0.0008 (10)	−0.0005 (10)
O01	0.007 (3)	0.010 (3)	0.008 (3)	0.004 (2)	−0.003 (2)	0.000 (2)
O02	0.004 (3)	0.014 (3)	0.008 (3)	0.000 (3)	−0.001 (2)	0.002 (3)
O03	0.002 (3)	0.010 (3)	0.010 (3)	0.002 (2)	0.001 (2)	−0.001 (2)
O04	0.011 (3)	0.009 (3)	0.014 (3)	0.007 (3)	−0.001 (3)	0.000 (3)
O05	0.007 (3)	0.011 (3)	0.010 (3)	0.003 (3)	0.002 (2)	0.001 (3)
O06	0.007 (3)	0.012 (3)	0.008 (3)	0.006 (3)	0.000 (2)	−0.004 (2)
O07	0.006 (3)	0.008 (3)	0.008 (3)	0.006 (2)	−0.002 (2)	−0.002 (2)
O08	0.009 (3)	0.006 (3)	0.008 (3)	0.003 (2)	−0.002 (2)	0.001 (2)
O09	0.015 (3)	0.005 (3)	0.010 (3)	0.002 (3)	−0.002 (3)	−0.002 (2)
O10	0.006 (3)	0.009 (3)	0.013 (3)	−0.001 (2)	0.001 (3)	0.005 (3)
O11	0.007 (3)	0.008 (3)	0.011 (3)	0.004 (2)	0.001 (2)	0.000 (2)
O12	0.013 (3)	0.006 (3)	0.013 (3)	0.005 (3)	0.001 (3)	0.002 (2)
O13	0.013 (3)	0.010 (3)	0.010 (3)	0.001 (3)	0.003 (3)	−0.004 (3)
O14	0.015 (3)	0.016 (3)	0.006 (3)	0.005 (3)	0.000 (3)	0.003 (3)
O15	0.004 (3)	0.008 (3)	0.010 (3)	0.002 (2)	0.002 (2)	0.000 (2)
O16	0.006 (3)	0.007 (3)	0.008 (3)	0.002 (2)	−0.002 (2)	0.002 (2)
O17	0.012 (3)	0.017 (3)	0.012 (3)	0.005 (3)	−0.006 (3)	−0.004 (3)
O18	0.007 (3)	0.011 (3)	0.016 (3)	0.006 (3)	−0.001 (3)	0.000 (3)
O19	0.007 (3)	0.004 (3)	0.011 (3)	0.001 (2)	0.002 (2)	−0.002 (2)
O20	0.008 (3)	0.008 (3)	0.005 (3)	0.002 (2)	−0.002 (2)	0.000 (2)
O21	0.012 (3)	0.005 (3)	0.009 (3)	0.002 (2)	−0.002 (3)	−0.001 (2)

O22	0.008 (3)	0.007 (3)	0.010 (3)	0.000 (2)	0.000 (2)	−0.004 (2)
O23	0.016 (3)	0.011 (3)	0.012 (3)	0.011 (3)	−0.005 (3)	−0.002 (3)
O24	0.013 (3)	0.012 (3)	0.008 (3)	0.006 (3)	−0.005 (3)	−0.002 (2)
O25	0.006 (3)	0.013 (3)	0.005 (3)	0.003 (2)	−0.003 (2)	−0.001 (2)
O26	0.008 (3)	0.011 (3)	0.016 (3)	0.005 (3)	0.000 (3)	0.003 (3)
O27	0.0082 (17)	0.0096 (17)	0.0109 (17)	0.0040 (12)	−0.0005 (12)	−0.0007 (12)
O28	0.007 (3)	0.003 (3)	0.011 (3)	0.001 (2)	0.002 (2)	0.000 (2)
O29	0.007 (3)	0.010 (3)	0.010 (3)	0.003 (2)	−0.002 (2)	0.004 (2)
O30	0.007 (3)	0.008 (3)	0.013 (3)	0.004 (2)	−0.003 (2)	−0.001 (2)
O31	0.009 (3)	0.007 (3)	0.010 (3)	0.000 (2)	0.001 (2)	0.000 (2)
O32	0.007 (3)	0.012 (3)	0.013 (3)	0.004 (3)	0.000 (3)	0.003 (3)
O33	0.011 (3)	0.009 (3)	0.013 (3)	0.000 (3)	0.006 (3)	−0.003 (3)
O34	0.004 (3)	0.009 (3)	0.010 (3)	0.000 (2)	−0.002 (2)	0.000 (2)
O35	0.012 (3)	0.010 (3)	0.008 (3)	0.007 (3)	−0.005 (2)	−0.004 (2)
O36	0.011 (3)	0.017 (4)	0.013 (3)	0.006 (3)	0.001 (3)	−0.007 (3)
O37	0.010 (3)	0.005 (3)	0.019 (4)	0.003 (2)	0.005 (3)	0.004 (3)
O38	0.010 (3)	0.013 (3)	0.013 (3)	0.010 (2)	−0.001 (2)	−0.002 (2)
O39	0.011 (3)	0.010 (3)	0.014 (3)	−0.002 (3)	−0.004 (3)	0.002 (3)
O40	0.007 (3)	0.010 (3)	0.007 (3)	0.005 (2)	0.001 (2)	0.001 (2)
O41	0.005 (3)	0.005 (3)	0.009 (3)	0.000 (2)	0.002 (2)	0.004 (2)
O42	0.008 (3)	0.012 (3)	0.014 (3)	0.003 (3)	0.003 (3)	0.000 (3)
O43	0.005 (3)	0.006 (3)	0.012 (3)	0.004 (2)	0.001 (2)	−0.001 (2)
O44	0.006 (3)	0.016 (3)	0.009 (3)	0.004 (3)	0.000 (2)	0.002 (3)
O45	0.005 (3)	0.005 (3)	0.009 (3)	0.001 (2)	−0.001 (2)	−0.003 (2)
O46	0.015 (4)	0.009 (3)	0.019 (4)	0.003 (3)	0.000 (3)	−0.002 (3)
O47	0.011 (3)	0.013 (3)	0.017 (4)	0.005 (3)	−0.002 (3)	0.003 (3)
O48	0.009 (3)	0.013 (3)	0.009 (3)	0.008 (3)	−0.003 (2)	−0.005 (3)
O49	0.008 (3)	0.007 (3)	0.016 (3)	0.001 (2)	0.007 (3)	0.000 (3)
O50	0.008 (3)	0.011 (3)	0.008 (3)	0.004 (2)	0.000 (2)	−0.002 (2)
O51	0.009 (3)	0.012 (3)	0.016 (3)	0.003 (3)	−0.001 (3)	0.002 (3)
O52	0.015 (3)	0.010 (3)	0.012 (3)	0.004 (3)	0.002 (3)	−0.001 (3)
O53	0.005 (3)	0.005 (3)	0.018 (3)	0.000 (2)	0.003 (2)	−0.002 (2)
O54	0.010 (3)	0.008 (3)	0.014 (3)	0.005 (3)	−0.001 (3)	−0.002 (3)
O55	0.012 (3)	0.014 (3)	0.010 (3)	0.003 (3)	−0.004 (3)	0.003 (3)
O56	0.016 (4)	0.014 (3)	0.009 (3)	0.005 (3)	0.001 (3)	0.003 (3)
O57	0.012 (3)	0.010 (3)	0.004 (3)	0.001 (2)	−0.001 (2)	−0.003 (2)
O58	0.013 (3)	0.009 (3)	0.006 (3)	0.002 (3)	0.004 (3)	0.002 (2)
O59	0.009 (3)	0.005 (3)	0.013 (3)	−0.002 (2)	0.006 (3)	−0.004 (2)
O60	0.008 (3)	0.017 (3)	0.013 (3)	0.008 (3)	0.003 (3)	−0.002 (3)
O61	0.007 (3)	0.013 (3)	0.009 (3)	0.003 (3)	0.001 (2)	−0.001 (3)

O62	0.008 (3)	0.009 (3)	0.011 (3)	0.006 (2)	0.001 (2)	0.001 (2)
O63	0.009 (3)	0.009 (3)	0.015 (3)	0.006 (3)	−0.001 (3)	0.001 (3)
O64	0.010 (3)	0.007 (3)	0.011 (3)	0.003 (2)	−0.003 (3)	0.004 (2)
O65	0.008 (3)	0.009 (3)	0.007 (3)	0.004 (2)	−0.003 (2)	−0.001 (2)
O66	0.010 (3)	0.011 (3)	0.014 (3)	0.005 (3)	0.002 (3)	0.000 (3)
O67	0.007 (3)	0.005 (3)	0.020 (4)	0.004 (2)	−0.001 (3)	−0.002 (3)
O68	0.008 (3)	0.006 (3)	0.015 (3)	0.003 (2)	0.003 (3)	0.002 (2)
O69	0.011 (3)	0.007 (3)	0.009 (3)	0.006 (2)	0.003 (2)	−0.002 (2)
O70	0.006 (3)	0.009 (3)	0.013 (3)	0.000 (2)	−0.003 (3)	−0.001 (3)
O71	0.010 (3)	0.006 (3)	0.012 (3)	0.002 (2)	0.000 (3)	0.001 (2)
O72	0.009 (3)	0.010 (3)	0.011 (3)	0.004 (2)	−0.004 (2)	0.000 (2)
O73	0.008 (3)	0.004 (3)	0.015 (3)	0.003 (2)	−0.002 (3)	0.002 (2)
O74	0.012 (3)	0.004 (3)	0.020 (4)	0.001 (3)	0.003 (3)	−0.002 (3)
O75	0.007 (3)	0.009 (3)	0.017 (3)	0.004 (2)	0.002 (3)	−0.002 (3)
O76	0.011 (3)	0.021 (4)	0.012 (3)	0.008 (3)	−0.005 (3)	−0.005 (3)
O77	0.011 (3)	0.012 (3)	0.008 (3)	0.002 (3)	0.000 (3)	−0.001 (3)
O78	0.014 (3)	0.013 (3)	0.007 (3)	0.008 (3)	0.004 (3)	0.002 (2)
O79	0.005 (3)	0.010 (3)	0.006 (3)	0.002 (2)	−0.001 (2)	0.000 (2)
O80	0.012 (3)	0.003 (3)	0.014 (3)	0.001 (2)	0.001 (3)	0.001 (2)
O81	0.009 (3)	0.016 (3)	0.011 (3)	0.005 (3)	−0.005 (3)	0.000 (3)
O82	0.009 (3)	0.009 (3)	0.012 (3)	0.004 (2)	−0.001 (3)	0.000 (2)
O83	0.011 (3)	0.012 (3)	0.015 (3)	0.003 (3)	−0.003 (3)	0.003 (3)
O84	0.007 (3)	0.005 (3)	0.013 (3)	−0.001 (2)	0.001 (3)	0.005 (2)
O85	0.012 (3)	0.009 (3)	0.014 (3)	0.003 (3)	−0.003 (3)	0.000 (3)
O86	0.014 (3)	0.013 (3)	0.011 (3)	0.007 (3)	0.000 (3)	0.006 (3)
O87	0.008 (3)	0.013 (3)	0.016 (3)	0.004 (3)	−0.001 (3)	−0.003 (3)
O88	0.015 (3)	0.009 (3)	0.012 (3)	0.006 (3)	−0.004 (3)	−0.001 (2)
O89	0.010 (3)	0.010 (3)	0.007 (3)	0.001 (3)	0.001 (2)	0.003 (2)
O90	0.016 (3)	0.010 (3)	0.012 (3)	0.009 (3)	−0.001 (3)	0.001 (3)
O91	0.012 (3)	0.015 (3)	0.019 (4)	0.008 (3)	0.002 (3)	0.000 (3)
O92	0.018 (4)	0.014 (3)	0.012 (3)	0.007 (3)	0.002 (3)	0.001 (3)
O93	0.012 (3)	0.011 (3)	0.007 (3)	0.006 (3)	0.001 (2)	−0.002 (2)
O94	0.021 (4)	0.009 (3)	0.011 (3)	0.002 (3)	0.008 (3)	0.003 (3)
O95	0.007 (3)	0.008 (3)	0.014 (3)	0.001 (2)	0.000 (3)	0.005 (3)
O96	0.019 (4)	0.009 (3)	0.012 (3)	−0.003 (3)	−0.004 (3)	−0.002 (3)

Table S4. Bond Lengths for $Ba_3[Al(PO_4)_3]$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ba(01)	O(01)[1]	2.815(8)	Ba(20)	O(43)[9]	2.981(8)
Ba(01)	O(07)	2.714(7)	Ba(20)	O(47)[13]	3.138(9)
Ba(01)	O(23)[1]	2.914(9)	Ba(20)	O(50)	2.731(8)
Ba(01)	O(25)[1]	2.794(8)	Ba(20)	O(77)[9]	2.970(8)
Ba(01)	O(31)[1]	2.940(8)	Ba(20)	O(93)[9]	2.926(8)
Ba(01)	O(56)	2.985(9)	Ba(20)	O(96)[9]	3.045(10)
Ba(01)	O(57)[1]	3.103(9)	Ba(21)	O(24)	2.961(8)
Ba(01)	O(70)[1]	3.054(8)	Ba(21)	O(34)[13]	2.784(8)
Ba(01)	O(96)[1]	2.808(8)	Ba(21)	O(39)[8]	3.097(9)
Ba(02)	O(10)[2]	3.046(8)	Ba(21)	O(42)[11]	2.720(8)
Ba(02)	O(14)[2]	2.838(9)	Ba(21)	O(56)[13]	3.084(9)
Ba(02)	O(22)[3]	2.975(8)	Ba(21)	O(82)[11]	3.089(8)
Ba(02)	O(41)[3]	2.848(8)	Ba(21)	O(83)[8]	2.752(9)
Ba(02)	O(49)[3]	2.892(8)	Ba(21)	O(86)	2.667(8)
Ba(02)	O(68)[3]	2.759(8)	Ba(22)	O(02)	2.711(8)
Ba(02)	O(69)	2.880(8)	Ba(22)	O(15)[6]	2.811(8)
Ba(02)	O(90)	2.706(8)	Ba(22)	O(25)	2.860(8)
Ba(03)	O(35)	2.815(8)	Ba(22)	O(45)[6]	2.717(8)
Ba(03)	O(36)	2.883(8)	Ba(22)	O(48)	2.820(8)
Ba(03)	O(39)	2.807(8)	Ba(22)	O(60)[6]	2.740(8)
Ba(03)	O(43)	2.702(7)	Ba(22)	O(63)	2.634(8)
Ba(03)	O(57)	3.111(9)	Ba(22)	O(70)	2.785(8)
Ba(03)	O(74)	2.678(8)	Ba(22)	O(90)[6]	3.075(8)
Ba(03)	O(82)[4]	2.680(8)	Ba(23)	O(04)[8]	2.902(8)
Ba(03)	O(85)[4]	2.806(9)	Ba(23)	O(15)[6]	2.791(8)
Ba(04)	O(14)	2.791(9)	Ba(23)	O(19)[6]	2.763(8)
Ba(04)	O(31)[1]	2.831(8)	Ba(23)	O(24)	2.645(8)
Ba(04)	O(33)	2.658(8)	Ba(23)	O(25)	2.892(8)
Ba(04)	O(36)	2.915(9)	Ba(23)	O(54)	2.726(8)
Ba(04)	O(41)[1]	2.888(8)	Ba(23)	O(76)[8]	3.112(10)
Ba(04)	O(53)[1]	2.694(8)	Ba(23)	O(92)[8]	3.086(9)
Ba(04)	O(62)[1]	3.036(8)	Ba(24)	O(29)[1]	2.882(8)
Ba(04)	O(91)[1]	2.966(9)	Ba(24)	O(30)[5]	2.760(8)
Ba(05)	O(08)[5]	2.746(8)	Ba(24)	O(34)[5]	3.110(8)
Ba(05)	O(40)[5]	2.886(8)	Ba(24)	O(38)	2.698(8)
Ba(05)	O(43)[5]	2.771(8)	Ba(24)	O(42)[1]	2.975(8)
Ba(05)	O(50)[3]	2.981(8)	Ba(24)	O(64)[3]	2.764(8)

Ba(05)	O(65)[5]	2.744(8)	Ba(24)	O(77)[15]	2.859(9)
Ba(05)	O(69)	2.695(7)	Ba(25)	O(07)[13]	2.921(7)
Ba(05)	O(75)[3]	2.772(8)	Ba(25)	O(09)[10]	2.886(9)
Ba(06)	O(02)	2.660(8)	Ba(25)	O(12)[10]	2.792(9)
Ba(06)	O(03)[6]	3.027(8)	Ba(25)	O(26)[10]	2.964(8)
Ba(06)	O(06)[6]	2.772(8)	Ba(25)	O(27)[13]	2.895(8)
Ba(06)	O(15)[6]	2.804(8)	Ba(25)	O(85)[10]	2.897(9)
Ba(06)	O(18)[6]	2.889(8)	Ba(25)	O(91)	2.733(9)
Ba(06)	O(28)[1]	2.685(7)	Ba(26)	O(04)[8]	2.693(9)
Ba(06)	O(41)[1]	2.868(8)	Ba(26)	O(18)[6]	3.034(8)
Ba(06)	O(44)	2.963(8)	Ba(26)	O(24)	3.006(8)
Ba(07)	O(10)[8]	2.782(9)	Ba(26)	O(26)[11]	2.906(9)
Ba(07)	O(19)[6]	2.719(8)	Ba(26)	O(72)[6]	2.912(8)
Ba(07)	O(29)[6]	2.830(8)	Ba(26)	O(81)	2.698(9)
Ba(07)	O(46)	2.604(9)	Ba(26)	O(82)[11]	2.743(8)
Ba(07)	O(49)[6]	2.648(8)	P(01)	O(08)	1.525(8)
Ba(07)	O(58)[8]	2.758(8)	P(01)	O(30)	1.515(8)
Ba(07)	O(84)[6]	2.878(8)	P(01)	O(40)	1.523(8)
Ba(08)	O(03)[8]	2.755(7)	P(01)	O(78)	1.575(8)
Ba(08)	O(11)[8]	2.797(8)	P(02)	O(07)	1.527(8)
Ba(08)	O(28)	2.648(8)	P(02)	O(27)	1.577(8)
Ba(08)	O(40)[9]	2.774(8)	P(02)	O(34)	1.539(8)
Ba(08)	O(55)[8]	2.715(8)	P(02)	O(56)	1.518(9)
Ba(08)	O(61)[8]	2.975(8)	P(03)	O(04)	1.529(8)
Ba(08)	O(71)[8]	3.089(8)	P(03)	O(14)	1.544(8)
Ba(11)	O(05)[2]	2.851(8)	P(03)	O(36)	1.521(9)
Ba(11)	O(10)[2]	2.800(8)	P(03)	O(76)	1.589(9)
Ba(11)	O(29)[3]	2.908(8)	P(04)	O(22)	1.521(8)
Ba(11)	O(37)[2]	2.785(8)	P(04)	O(28)	1.536(8)
Ba(11)	O(47)[2]	2.964(9)	P(04)	O(41)	1.526(8)
Ba(11)	O(50)[3]	2.766(8)	P(04)	O(73)	1.587(8)
Ba(11)	O(60)	2.676(9)	P(05)	O(31)	1.526(8)
Ba(11)	O(69)	2.999(8)	P(05)	O(72)	1.603(9)
Ba(12)	O(06)[6]	2.698(8)	P(05)	O(91)	1.507(9)
Ba(12)	O(21)	2.830(8)	P(05)	O(96)	1.524(10)
Ba(12)	O(33)	2.790(8)	P(06)	O(01)	1.525(8)
Ba(12)	O(53)[1]	2.721(8)	P(06)	O(16)	1.585(8)
Ba(12)	O(54)[1]	2.706(8)	P(06)	O(43)	1.534(8)
Ba(12)	O(56)	2.661(9)	P(06)	O(65)	1.530(8)
Ba(12)	O(83)[6]	2.708(9)	P(07)	O(21)	1.567(8)

Ba(12)	O(88)^{6}	2.855(8)	P(07)	O(33)	1.516(8)
Ba(13)	O(05)	2.905(8)	P(07)	O(44)	1.571(9)
Ba(13)	O(17)	2.743(9)	P(07)	O(74)	1.499(9)
Ba(13)	O(31)	2.732(8)	P(08)	O(67)	1.564(8)
Ba(13)	O(51)	2.743(9)	P(08)	O(77)	1.524(9)
Ba(13)	O(52)	2.626(8)	P(08)	O(87)	1.527(8)
Ba(13)	O(63)	2.622(8)	P(08)	O(93)	1.559(8)
Ba(13)	O(70)	2.694(8)	P(09)	O(06)	1.524(8)
Ba(13)	O(72)	3.146(8)	P(09)	O(18)	1.517(8)
Ba(13)	O(95)	2.911(8)	P(09)	O(52)	1.519(9)
Ba(14)	O(09)^{10}	2.742(8)	P(09)	O(88)	1.601(9)
Ba(14)	O(26)^{10}	2.815(9)	P(10)	O(02)	1.498(8)
Ba(14)	O(55)^{10}	2.716(9)	P(10)	O(35)	1.567(8)
Ba(14)	O(59)^{10}	2.677(7)	P(10)	O(57)	1.557(8)
Ba(14)	O(66)^{10}	2.951(8)	P(10)	O(70)	1.521(8)
Ba(14)	O(77)	2.883(8)	P(11)	O(09)	1.535(9)
Ba(14)	O(87)	2.659(8)	P(11)	O(12)	1.522(8)
Ba(14)	O(89)^{10}	2.909(8)	P(11)	O(47)	1.525(9)
Ba(15)	O(08)^{9}	2.701(8)	P(11)	O(89)	1.598(8)
Ba(15)	O(12)	2.650(8)	P(12)	O(03)	1.539(8)
Ba(15)	O(20)	2.826(8)	P(12)	O(15)	1.527(8)
Ba(15)	O(22)	2.668(8)	P(12)	O(19)	1.531(8)
Ba(15)	O(30)^{9}	2.785(8)	P(12)	O(45)	1.584(8)
Ba(15)	O(64)	2.820(8)	P(13)	O(20)	1.567(8)
Ba(15)	O(68)	2.674(8)	P(13)	O(46)	1.505(9)
Ba(16)	O(16)	2.702(8)	P(13)	O(64)	1.512(9)
Ba(16)	O(40)	2.881(8)	P(13)	O(79)	1.557(8)
Ba(16)	O(59)^{11}	2.722(8)	P(14)	O(13)	1.565(9)
Ba(16)	O(65)	2.904(8)	P(14)	O(51)	1.514(9)
Ba(16)	O(78)	2.804(8)	P(14)	O(62)	1.552(8)
Ba(16)	O(80)^{11}	2.787(8)	P(14)	O(63)	1.494(9)
Ba(16)	O(81)	2.749(8)	P(15)	O(11)	1.585(8)
Ba(16)	O(86)	2.943(9)	P(15)	O(60)	1.527(8)
Ba(16)	O(87)^{6}	2.980(8)	P(15)	O(69)	1.533(8)
Ba(17)	O(01)^{5}	2.968(8)	P(15)	O(90)	1.516(9)
Ba(17)	O(07)^{12}	2.712(8)	P(16)	O(25)	1.523(8)
Ba(17)	O(12)^{2}	2.865(8)	P(16)	O(48)	1.578(8)
Ba(17)	O(34)^{12}	2.840(8)	P(16)	O(53)	1.518(8)
Ba(17)	O(47)^{2}	2.964(9)	P(16)	O(54)	1.537(9)
Ba(17)	O(64)^{2}	2.910(8)	P(17)	O(37)	1.598(8)

Ba(17)	O(65)[5]	2.823(8)	P(17)	O(38)	1.512(8)
Ba(17)	O(79)[2]	2.948(8)	P(17)	O(55)	1.522(9)
Ba(17)	O(80)	2.671(8)	P(17)	O(61)	1.525(8)
Ba(18)	O(05)	2.938(8)	P(18)	O(29)	1.537(8)
Ba(18)	O(06)	2.805(8)	P(18)	O(42)	1.507(9)
Ba(18)	O(28)[3]	2.952(8)	P(18)	O(50)	1.527(9)
Ba(18)	O(38)	2.739(8)	P(18)	O(75)	1.608(8)
Ba(18)	O(52)	2.878(8)	P(19)	O(05)	1.519(9)
Ba(18)	O(58)	2.799(9)	P(19)	O(10)	1.526(8)
Ba(18)	O(61)	2.838(8)	P(19)	O(17)	1.580(9)
Ba(18)	O(73)[3]	2.840(8)	P(19)	O(58)	1.529(9)
Ba(19)	O(03)	2.813(8)	P(20)	O(39)	1.515(9)
Ba(19)	O(04)[13]	2.845(8)	P(20)	O(83)	1.506(9)
Ba(19)	O(14)[13]	3.001(9)	P(20)	O(92)	1.568(9)
Ba(19)	O(18)	3.008(9)	P(20)	O(95)	1.562(9)
Ba(19)	O(19)	3.075(8)	P(21)	O(59)	1.519(8)
Ba(19)	O(32)	3.039(8)	P(21)	O(71)	1.548(8)
Ba(19)	O(51)	2.697(8)	P(21)	O(80)	1.502(9)
Ba(19)	O(52)	3.029(9)	P(21)	O(84)	1.585(9)
Ba(19)	O(61)	2.812(8)	P(22)	O(32)	1.574(9)
Ba(20)	O(01)[9]	2.861(8)	P(22)	O(49)	1.503(8)
Ba(20)	O(09)[13]	2.769(9)	P(22)	O(66)	1.554(9)
Ba(20)	O(39)[9]	3.020(9)	P(22)	O(68)	1.519(8)
Al(4)	O(20)	1.738(8)	Al(1)	O(13)	1.716(9)
Al(4)	O(48)	1.722(9)	Al(1)	O(32)	1.741(8)
Al(4)	O(62)	1.763(9)	Al(1)	O(37)	1.731(9)
Al(4)	O(73)	1.718(8)	Al(1)	O(89)	1.720(9)
P(24)	O(26)	1.524(9)	Al(2)	O(66)	1.760(9)
P(24)	O(82)	1.535(9)	Al(2)	O(75)	1.714(9)
P(24)	O(85)	1.533(9)	Al(2)	O(84)	1.735(8)
P(24)	O(94)	1.573(8)	Al(2)	O(94)	1.724(9)
Al(5)	O(17)	1.714(9)	Al(3)	O(11)	1.744(8)
Al(5)	O(35)	1.712(8)	Al(3)	O(45)	1.738(8)
Al(5)	O(76)	1.716(9)	Al(3)	O(71)	1.753(8)
Al(5)	O(92)	1.746(9)	Al(3)	O(79)[2]	1.741(8)
Al(6)	O(16)	1.738(8)	P(23)	O(23)	1.595(9)
Al(6)	O(23)	1.733(9)	P(23)	O(24)	1.523(9)
Al(6)	O(44)	1.735(8)	P(23)	O(81)	1.524(8)
Al(6)	O(57)	1.755(8)	P(23)	O(86)	1.521(9)
Al(7)	O(72)	1.739(9)	Al(8)	O(27)	1.739(9)

Al(7)	O(88)	1.715(9)	Al(8)	O(67)[6]	1.749(8)
Al(7)	O(93)	1.735(8)	Al(8)	O(78)	1.714(8)
Al(7)	O(95)	1.770(8)	Al(8)	O(21)	1.740(9)

[1]-1+X,+Y,+Z; [2]1+X,1+Y,+Z; [3]+X,1+Y,+Z; [4]-1+X,+Y,-1+Z; [5]1+X,1+Y,1+Z; [6]-1+X,-1+Y,+Z; [7]-1+X,-2+Y,+Z; [8]+X,-1+Y,+Z; [9]1+X,+Y,1+Z; [10]+X,+Y,-1+Z; [11]-1+X,-1+Y,-1+Z; [12]2+X,1+Y,1+Z; [13]1+X,+Y,+Z; [14]+X,-1+Y,-1+Z; [15]+X,+Y,1+Z

Table S5. Crystal data and structure refinement for $Ba_3[Al(PO_4)_3]$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O(01)^{1}	Ba(01)	O(23)^{1}	79.2(2)	O(25)	Ba(23)	O(92)^{8}	122.6(2)
O(01)^{1}	Ba(01)	O(31)^{1}	119.6(2)	O(54)	Ba(23)	O(04)^{8}	163.9(2)
O(01)^{1}	Ba(01)	O(56)	103.6(2)	O(54)	Ba(23)	O(15)^{5}	105.7(2)
O(01)^{1}	Ba(01)	O(57)^{1}	62.1(2)	O(54)	Ba(23)	O(19)^{5}	107.3(2)
O(01)^{1}	Ba(01)	O(70)^{1}	101.4(2)	O(54)	Ba(23)	O(25)	53.1(2)
O(07)	Ba(01)	O(01)^{1}	63.5(2)	O(54)	Ba(23)	O(76)^{8}	115.1(2)
O(07)	Ba(01)	O(23)^{1}	110.5(2)	O(54)	Ba(23)	O(92)^{8}	81.7(2)
O(07)	Ba(01)	O(25)^{1}	131.0(2)	O(92)^{8}	Ba(23)	O(76)^{8}	53.0(2)
O(07)	Ba(01)	O(31)^{1}	105.2(2)	O(29)^{1}	Ba(24)	O(34)^{6}	113.8(2)
O(07)	Ba(01)	O(56)	51.6(2)	O(29)^{1}	Ba(24)	O(42)^{1}	50.7(2)
O(07)	Ba(01)	O(57)^{1}	125.2(2)	O(30)^{6}	Ba(24)	O(29)^{1}	151.3(2)
O(07)	Ba(01)	O(70)^{1}	154.2(2)	O(30)^{6}	Ba(24)	O(34)^{6}	91.3(2)
O(07)	Ba(01)	O(96)^{1}	68.4(2)	O(30)^{6}	Ba(24)	O(42)^{1}	157.6(2)
O(23)^{1}	Ba(01)	O(31)^{1}	144.3(2)	O(30)^{6}	Ba(24)	O(64)^{2}	69.2(2)
O(23)^{1}	Ba(01)	O(56)	88.9(2)	O(30)^{6}	Ba(24)	O(77)^{15}	99.5(2)
O(23)^{1}	Ba(01)	O(57)^{1}	54.0(2)	O(38)	Ba(24)	O(29)^{1}	66.1(2)
O(23)^{1}	Ba(01)	O(70)^{1}	85.1(2)	O(38)	Ba(24)	O(30)^{6}	86.0(2)
O(25)^{1}	Ba(01)	O(01)^{1}	145.1(2)	O(38)	Ba(24)	O(34)^{6}	164.6(2)
O(25)^{1}	Ba(01)	O(23)^{1}	66.0(2)	O(38)	Ba(24)	O(42)^{1}	113.6(2)
O(25)^{1}	Ba(01)	O(31)^{1}	89.4(2)	O(38)	Ba(24)	O(64)^{2}	100.7(2)
O(25)^{1}	Ba(01)	O(56)	79.4(2)	O(38)	Ba(24)	O(77)^{15}	95.7(2)
O(25)^{1}	Ba(01)	O(57)^{1}	93.4(2)	O(42)^{1}	Ba(24)	O(34)^{6}	72.7(2)
O(25)^{1}	Ba(01)	O(70)^{1}	73.7(2)	O(64)^{2}	Ba(24)	O(29)^{1}	108.1(2)
O(25)^{1}	Ba(01)	O(96)^{1}	141.5(2)	O(64)^{2}	Ba(24)	O(34)^{6}	64.3(2)
O(31)^{1}	Ba(01)	O(56)	112.7(2)	O(64)^{2}	Ba(24)	O(42)^{1}	114.9(2)
O(31)^{1}	Ba(01)	O(57)^{1}	105.4(2)	O(64)^{2}	Ba(24)	O(77)^{15}	159.2(2)
O(31)^{1}	Ba(01)	O(70)^{1}	62.5(2)	O(77)^{15}	Ba(24)	O(29)^{1}	90.2(2)
O(56)	Ba(01)	O(57)^{1}	141.0(2)	O(77)^{15}	Ba(24)	O(34)^{6}	99.7(2)
O(56)	Ba(01)	O(70)^{1}	152.7(2)	O(77)^{15}	Ba(24)	O(42)^{1}	68.9(2)
O(70)^{1}	Ba(01)	O(57)^{1}	47.7(2)	O(07)^{13}	Ba(25)	O(26)^{10}	139.8(2)
O(96)^{1}	Ba(01)	O(01)^{1}	70.5(2)	O(07)^{13}	Ba(25)	O(74)^{13}	108.6(2)
O(96)^{1}	Ba(01)	O(23)^{1}	146.5(3)	O(07)^{13}	Ba(25)	O(96)	61.0(2)
O(96)^{1}	Ba(01)	O(31)^{1}	52.1(2)	O(09)^{10}	Ba(25)	O(07)^{13}	81.9(2)
O(96)^{1}	Ba(01)	O(56)	111.5(3)	O(09)^{10}	Ba(25)	O(26)^{10}	65.9(2)
O(96)^{1}	Ba(01)	O(57)^{1}	98.0(3)	O(09)^{10}	Ba(25)	O(27)^{13}	125.3(2)
O(96)^{1}	Ba(01)	O(70)^{1}	87.2(2)	O(09)^{10}	Ba(25)	O(74)^{13}	167.8(2)
O(14)^{3}	Ba(02)	O(10)^{3}	104.1(2)	O(09)^{10}	Ba(25)	O(85)^{10}	103.9(2)

O(14)^{3}	Ba(02)	O(22)^{2}	109.8(2)	O(09)^{10}	Ba(25)	O(96)	61.6(2)
O(14)^{3}	Ba(02)	O(41)^{2}	75.7(2)	O(12)^{10}	Ba(25)	O(07)^{13}	62.4(2)
O(14)^{3}	Ba(02)	O(49)^{2}	76.4(3)	O(12)^{10}	Ba(25)	O(09)^{10}	52.4(2)
O(14)^{3}	Ba(02)	O(69)	166.5(2)	O(12)^{10}	Ba(25)	O(26)^{10}	109.4(2)
O(22)^{2}	Ba(02)	O(10)^{3}	145.9(2)	O(12)^{10}	Ba(25)	O(27)^{13}	80.1(2)
O(41)^{2}	Ba(02)	O(10)^{3}	146.6(2)	O(12)^{10}	Ba(25)	O(74)^{13}	137.7(2)
O(41)^{2}	Ba(02)	O(22)^{2}	51.1(2)	O(12)^{10}	Ba(25)	O(85)^{10}	113.2(2)
O(41)^{2}	Ba(02)	O(49)^{2}	139.6(2)	O(12)^{10}	Ba(25)	O(96)	94.9(2)
O(41)^{2}	Ba(02)	O(69)	117.5(2)	O(26)^{10}	Ba(25)	O(74)^{13}	101.9(2)
O(49)^{2}	Ba(02)	O(10)^{3}	69.2(2)	O(26)^{10}	Ba(25)	O(96)	82.0(2)
O(49)^{2}	Ba(02)	O(22)^{2}	114.7(2)	O(27)^{13}	Ba(25)	O(07)^{13}	49.6(2)
O(68)^{2}	Ba(02)	O(10)^{3}	110.7(2)	O(27)^{13}	Ba(25)	O(26)^{10}	168.8(2)
O(68)^{2}	Ba(02)	O(14)^{3}	96.2(2)	O(27)^{13}	Ba(25)	O(74)^{13}	66.9(2)
O(68)^{2}	Ba(02)	O(22)^{2}	62.1(2)	O(27)^{13}	Ba(25)	O(85)^{10}	120.5(2)
O(68)^{2}	Ba(02)	O(41)^{2}	102.4(2)	O(27)^{13}	Ba(25)	O(96)	103.6(2)
O(68)^{2}	Ba(02)	O(49)^{2}	52.7(2)	O(85)^{10}	Ba(25)	O(07)^{13}	168.7(2)
O(68)^{2}	Ba(02)	O(69)	84.1(2)	O(85)^{10}	Ba(25)	O(26)^{10}	50.8(2)
O(69)	Ba(02)	O(10)^{3}	63.6(2)	O(85)^{10}	Ba(25)	O(74)^{13}	66.9(2)
O(69)	Ba(02)	O(22)^{2}	82.3(2)	O(85)^{10}	Ba(25)	O(96)	130.3(2)
O(69)	Ba(02)	O(49)^{2}	93.4(2)	O(91)	Ba(25)	O(07)^{13}	96.7(2)
O(90)	Ba(02)	O(10)^{3}	86.0(2)	O(91)	Ba(25)	O(09)^{10}	99.8(2)
O(90)	Ba(02)	O(14)^{3}	134.1(3)	O(91)	Ba(25)	O(12)^{10}	145.1(2)
O(90)	Ba(02)	O(22)^{2}	73.6(2)	O(91)	Ba(25)	O(26)^{10}	67.5(3)
O(90)	Ba(02)	O(41)^{2}	72.6(2)	O(91)	Ba(25)	O(27)^{13}	108.3(2)
O(90)	Ba(02)	O(49)^{2}	145.9(3)	O(91)	Ba(25)	O(74)^{13}	73.3(2)
O(90)	Ba(02)	O(68)^{2}	122.3(2)	O(91)	Ba(25)	O(85)^{10}	91.9(3)
O(90)	Ba(02)	O(69)	53.8(2)	O(91)	Ba(25)	O(96)	50.4(2)
O(35)	Ba(03)	O(36)	64.7(2)	O(96)	Ba(25)	O(74)^{13}	117.4(2)
O(35)	Ba(03)	O(57)	47.8(2)	O(04)^{8}	Ba(26)	O(18)^{5}	63.0(2)
O(36)	Ba(03)	O(57)	104.6(2)	O(04)^{8}	Ba(26)	O(24)	75.3(2)
O(39)	Ba(03)	O(35)	75.5(2)	O(04)^{8}	Ba(26)	O(26)^{11}	142.7(2)
O(39)	Ba(03)	O(36)	110.5(3)	O(04)^{8}	Ba(26)	O(72)^{5}	98.8(2)
O(39)	Ba(03)	O(57)	83.9(2)	O(04)^{8}	Ba(26)	O(81)	115.4(2)
O(43)	Ba(03)	O(35)	111.6(2)	O(04)^{8}	Ba(26)	O(82)^{11}	99.9(2)
O(43)	Ba(03)	O(36)	173.6(3)	O(04)^{8}	Ba(26)	O(91)^{5}	92.9(2)
O(43)	Ba(03)	O(39)	72.6(2)	O(18)^{5}	Ba(26)	O(91)^{5}	114.8(2)
O(43)	Ba(03)	O(57)	69.8(2)	O(24)	Ba(26)	O(18)^{5}	91.8(2)
O(43)	Ba(03)	O(85)^{4}	75.5(2)	O(24)	Ba(26)	O(91)^{5}	142.2(2)
O(74)	Ba(03)	O(35)	103.5(3)	O(26)^{11}	Ba(26)	O(18)^{5}	150.8(2)
O(74)	Ba(03)	O(36)	83.8(3)	O(26)^{11}	Ba(26)	O(24)	107.0(2)

O(74)	Ba(03)	O(39)	162.6(3)
O(74)	Ba(03)	O(43)	92.2(2)
O(74)	Ba(03)	O(57)	82.9(2)
O(74)	Ba(03)	O(82)^{4}	116.1(3)
O(74)	Ba(03)	O(85)^{4}	77.1(3)
O(82)^{4}	Ba(03)	O(35)	119.3(2)
O(82)^{4}	Ba(03)	O(36)	75.5(3)
O(82)^{4}	Ba(03)	O(39)	78.2(3)
O(82)^{4}	Ba(03)	O(43)	110.8(2)
O(82)^{4}	Ba(03)	O(57)	160.7(2)
O(82)^{4}	Ba(03)	O(85)^{4}	55.0(2)
O(85)^{4}	Ba(03)	O(35)	172.8(2)
O(85)^{4}	Ba(03)	O(36)	108.4(3)
O(85)^{4}	Ba(03)	O(39)	106.2(2)
O(85)^{4}	Ba(03)	O(57)	139.0(2)
O(14)	Ba(04)	O(31)^{1}	110.0(2)
O(14)	Ba(04)	O(36)	52.7(2)
O(14)	Ba(04)	O(41)^{1}	75.8(2)
O(14)	Ba(04)	O(62)^{1}	76.0(2)
O(14)	Ba(04)	O(91)^{1}	101.5(2)
O(31)^{1}	Ba(04)	O(36)	106.1(2)
O(31)^{1}	Ba(04)	O(41)^{1}	150.7(2)
O(31)^{1}	Ba(04)	O(62)^{1}	87.3(2)
O(31)^{1}	Ba(04)	O(91)^{1}	50.5(2)
O(33)	Ba(04)	O(14)	127.6(3)
O(33)	Ba(04)	O(31)^{1}	118.1(3)
O(33)	Ba(04)	O(36)	93.4(2)
O(33)	Ba(04)	O(41)^{1}	72.5(3)
O(33)	Ba(04)	O(53)^{1}	69.7(2)
O(33)	Ba(04)	O(62)^{1}	123.9(2)
O(33)	Ba(04)	O(91)^{1}	93.8(3)
O(36)	Ba(04)	O(62)^{1}	128.7(2)
O(36)	Ba(04)	O(91)^{1}	63.6(3)
O(41)^{1}	Ba(04)	O(36)	100.0(2)
O(41)^{1}	Ba(04)	O(62)^{1}	65.8(2)
O(41)^{1}	Ba(04)	O(91)^{1}	158.5(2)
O(53)^{1}	Ba(04)	O(14)	152.1(2)
O(53)^{1}	Ba(04)	O(31)^{1}	69.0(2)
O(53)^{1}	Ba(04)	O(36)	155.1(2)
O(53)^{1}	Ba(04)	O(41)^{1}	92.4(2)
O(26)^{11}	Ba(26)	O(72)^{5}	84.3(2)
O(26)^{11}	Ba(26)	O(91)^{5}	62.0(2)
O(72)^{5}	Ba(26)	O(18)^{5}	75.8(2)
O(72)^{5}	Ba(26)	O(24)	167.7(2)
O(72)^{5}	Ba(26)	O(91)^{5}	47.5(2)
O(81)	Ba(26)	O(18)^{5}	82.4(2)
O(81)	Ba(26)	O(24)	51.9(2)
O(81)	Ba(26)	O(26)^{11}	91.8(2)
O(81)	Ba(26)	O(72)^{5}	124.5(2)
O(81)	Ba(26)	O(82)^{11}	89.2(2)
O(81)	Ba(26)	O(91)^{5}	151.6(2)
O(82)^{11}	Ba(26)	O(18)^{5}	154.4(2)
O(82)^{11}	Ba(26)	O(24)	64.3(2)
O(82)^{11}	Ba(26)	O(26)^{11}	53.1(2)
O(82)^{11}	Ba(26)	O(72)^{5}	127.8(2)
O(82)^{11}	Ba(26)	O(91)^{5}	83.2(2)
O(08)	P(01)	O(78)	109.2(4)
O(30)	P(01)	O(08)	110.8(5)
O(30)	P(01)	O(40)	112.4(5)
O(30)	P(01)	O(78)	109.7(5)
O(40)	P(01)	O(08)	110.2(4)
O(40)	P(01)	O(78)	104.3(4)
O(07)	P(02)	O(27)	103.6(4)
O(07)	P(02)	O(34)	112.7(5)
O(34)	P(02)	O(27)	109.0(4)
O(56)	P(02)	O(07)	110.0(5)
O(56)	P(02)	O(27)	110.3(5)
O(56)	P(02)	O(34)	111.1(5)
O(04)	P(03)	O(14)	110.8(5)
O(04)	P(03)	O(76)	106.1(5)
O(14)	P(03)	O(76)	106.1(5)
O(36)	P(03)	O(04)	112.0(5)
O(36)	P(03)	O(14)	111.7(5)
O(36)	P(03)	O(76)	109.8(5)
O(22)	P(04)	O(28)	110.7(5)
O(22)	P(04)	O(41)	111.3(4)
O(22)	P(04)	O(73)	110.0(4)
O(28)	P(04)	O(73)	103.7(4)
O(41)	P(04)	O(28)	112.0(4)
O(41)	P(04)	O(73)	108.8(4)

O(53)[1]	Ba(04)	O(62)[1]	76.1(2)	O(31)	P(05)	O(72)	105.9(4)
O(53)[1]	Ba(04)	O(91)[1]	98.4(3)	O(91)	P(05)	O(31)	109.3(5)
O(91)[1]	Ba(04)	O(62)[1]	134.9(2)	O(91)	P(05)	O(72)	106.5(5)
O(08)[6]	Ba(05)	O(40)[6]	52.6(2)	O(91)	P(05)	O(96)	114.4(5)
O(08)[6]	Ba(05)	O(43)[6]	108.1(2)	O(96)	P(05)	O(31)	111.9(5)
O(08)[6]	Ba(05)	O(50)[2]	164.4(2)	O(96)	P(05)	O(72)	108.3(5)
O(08)[6]	Ba(05)	O(75)[2]	117.1(2)	O(01)	P(06)	O(16)	111.4(4)
O(08)[6]	Ba(05)	O(85)[2]	67.1(2)	O(01)	P(06)	O(43)	110.5(4)
O(40)[6]	Ba(05)	O(50)[2]	142.3(2)	O(01)	P(06)	O(65)	111.5(4)
O(40)[6]	Ba(05)	O(85)[2]	114.3(2)	O(43)	P(06)	O(16)	108.5(4)
O(43)[6]	Ba(05)	O(40)[6]	107.1(2)	O(65)	P(06)	O(16)	103.5(4)
O(43)[6]	Ba(05)	O(50)[2]	66.6(2)	O(65)	P(06)	O(43)	111.3(5)
O(43)[6]	Ba(05)	O(75)[2]	91.0(2)	O(21)	P(07)	O(44)	104.1(5)
O(43)[6]	Ba(05)	O(85)[2]	67.1(2)	O(33)	P(07)	O(21)	106.4(5)
O(50)[2]	Ba(05)	O(85)[2]	97.7(2)	O(33)	P(07)	O(44)	106.3(5)
O(65)[6]	Ba(05)	O(08)[6]	106.1(2)	O(74)	P(07)	O(21)	110.8(5)
O(65)[6]	Ba(05)	O(40)[6]	65.8(2)	O(74)	P(07)	O(33)	115.6(5)
O(65)[6]	Ba(05)	O(43)[6]	54.6(2)	O(74)	P(07)	O(44)	112.7(5)
O(65)[6]	Ba(05)	O(50)[2]	83.0(2)	O(77)	P(08)	O(67)	109.3(5)
O(65)[6]	Ba(05)	O(75)[2]	131.9(2)	O(77)	P(08)	O(87)	113.5(5)
O(65)[6]	Ba(05)	O(85)[2]	115.8(2)	O(77)	P(08)	O(93)	105.6(5)
O(69)	Ba(05)	O(08)[6]	112.3(2)	O(87)	P(08)	O(67)	110.0(5)
O(69)	Ba(05)	O(40)[6]	86.2(2)	O(87)	P(08)	O(93)	112.1(5)
O(69)	Ba(05)	O(43)[6]	136.8(2)	O(93)	P(08)	O(67)	106.0(5)
O(69)	Ba(05)	O(50)[2]	77.9(2)	O(06)	P(09)	O(88)	104.5(5)
O(69)	Ba(05)	O(65)[6]	98.9(2)	O(18)	P(09)	O(06)	113.4(5)
O(69)	Ba(05)	O(75)[2]	84.1(2)	O(18)	P(09)	O(52)	110.8(5)
O(69)	Ba(05)	O(85)[2]	144.5(2)	O(18)	P(09)	O(88)	109.1(5)
O(75)[2]	Ba(05)	O(40)[6]	161.0(2)	O(52)	P(09)	O(06)	108.4(5)
O(75)[2]	Ba(05)	O(50)[2]	50.4(2)	O(52)	P(09)	O(88)	110.4(5)
O(75)[2]	Ba(05)	O(85)[2]	67.2(2)	O(02)	P(10)	O(35)	110.7(5)
O(02)	Ba(06)	O(03)[5]	111.6(2)	O(02)	P(10)	O(57)	111.2(5)
O(02)	Ba(06)	O(06)[5]	150.3(2)	O(02)	P(10)	O(70)	112.3(5)
O(02)	Ba(06)	O(15)[5]	73.3(2)	O(57)	P(10)	O(35)	101.4(5)
O(02)	Ba(06)	O(18)[5]	130.0(2)	O(70)	P(10)	O(35)	112.8(5)
O(02)	Ba(06)	O(28)[1]	130.4(2)	O(70)	P(10)	O(57)	107.9(5)
O(02)	Ba(06)	O(33)	89.6(2)	O(09)	P(11)	O(89)	105.0(5)
O(02)	Ba(06)	O(41)[1]	90.5(2)	O(12)	P(11)	O(09)	110.3(5)
O(02)	Ba(06)	O(44)	64.5(2)	O(12)	P(11)	O(47)	112.4(5)
O(03)[5]	Ba(06)	O(33)	157.92(19)	O(12)	P(11)	O(89)	104.7(5)

O(06)[5]	Ba(06)	O(03)[5]	97.9(2)	O(47)	P(11)	O(09)	112.7(5)
O(06)[5]	Ba(06)	O(15)[5]	127.1(2)	O(47)	P(11)	O(89)	111.2(5)
O(06)[5]	Ba(06)	O(18)[5]	53.3(2)	O(03)	P(12)	O(45)	110.7(4)
O(06)[5]	Ba(06)	O(33)	61.6(2)	O(15)	P(12)	O(03)	110.5(4)
O(06)[5]	Ba(06)	O(41)[1]	83.4(2)	O(15)	P(12)	O(19)	111.0(4)
O(06)[5]	Ba(06)	O(44)	88.4(2)	O(15)	P(12)	O(45)	104.1(4)
O(15)[5]	Ba(06)	O(03)[5]	51.0(2)	O(19)	P(12)	O(03)	112.0(4)
O(15)[5]	Ba(06)	O(18)[5]	75.8(2)	O(19)	P(12)	O(45)	108.2(4)
O(15)[5]	Ba(06)	O(33)	147.5(2)	O(46)	P(13)	O(20)	111.6(5)
O(15)[5]	Ba(06)	O(41)[1]	141.3(2)	O(46)	P(13)	O(64)	114.6(5)
O(15)[5]	Ba(06)	O(44)	101.6(2)	O(46)	P(13)	O(79)	112.1(5)
O(18)[5]	Ba(06)	O(03)[5]	75.2(2)	O(64)	P(13)	O(20)	107.1(4)
O(18)[5]	Ba(06)	O(33)	96.3(2)	O(64)	P(13)	O(79)	106.1(5)
O(18)[5]	Ba(06)	O(44)	84.9(2)	O(79)	P(13)	O(20)	104.7(4)
O(28)[1]	Ba(06)	O(03)[5]	60.8(2)	O(51)	P(14)	O(13)	111.5(5)
O(28)[1]	Ba(06)	O(06)[5]	67.3(2)	O(51)	P(14)	O(62)	109.2(5)
O(28)[1]	Ba(06)	O(15)[5]	111.1(2)	O(62)	P(14)	O(13)	105.6(5)
O(28)[1]	Ba(06)	O(18)[5]	97.1(2)	O(63)	P(14)	O(13)	109.8(5)
O(28)[1]	Ba(06)	O(33)	101.1(2)	O(63)	P(14)	O(51)	111.3(5)
O(28)[1]	Ba(06)	O(41)[1]	54.3(2)	O(63)	P(14)	O(62)	109.3(5)
O(28)[1]	Ba(06)	O(44)	146.7(2)	O(60)	P(15)	O(11)	105.4(5)
O(41)[1]	Ba(06)	O(03)[5]	108.3(2)	O(60)	P(15)	O(69)	111.0(5)
O(41)[1]	Ba(06)	O(18)[5]	136.2(2)	O(69)	P(15)	O(11)	107.9(4)
O(41)[1]	Ba(06)	O(33)	63.7(2)	O(90)	P(15)	O(11)	108.7(5)
O(41)[1]	Ba(06)	O(44)	102.5(2)	O(90)	P(15)	O(60)	111.2(5)
O(44)	Ba(06)	O(03)[5]	149.1(2)	O(90)	P(15)	O(69)	112.2(5)
O(44)	Ba(06)	O(33)	45.9(2)	O(25)	P(16)	O(48)	105.1(4)
O(10)[8]	Ba(07)	O(29)[5]	71.7(2)	O(25)	P(16)	O(54)	110.5(5)
O(10)[8]	Ba(07)	O(84)[5]	124.5(2)	O(53)	P(16)	O(25)	112.1(5)
O(19)[5]	Ba(07)	O(10)[8]	108.4(2)	O(53)	P(16)	O(48)	110.8(5)
O(19)[5]	Ba(07)	O(29)[5]	179.7(2)	O(53)	P(16)	O(54)	110.3(5)
O(19)[5]	Ba(07)	O(58)[8]	80.8(2)	O(54)	P(16)	O(48)	107.7(5)
O(19)[5]	Ba(07)	O(84)[5]	110.3(2)	O(38)	P(17)	O(37)	109.0(5)
O(29)[5]	Ba(07)	O(84)[5]	69.8(2)	O(38)	P(17)	O(55)	110.4(5)
O(46)	Ba(07)	O(10)[8]	124.5(3)	O(38)	P(17)	O(61)	110.1(5)
O(46)	Ba(07)	O(19)[5]	97.9(3)	O(55)	P(17)	O(37)	107.3(5)
O(46)	Ba(07)	O(29)[5]	81.8(3)	O(55)	P(17)	O(61)	111.4(5)
O(46)	Ba(07)	O(49)[5]	158.2(3)	O(61)	P(17)	O(37)	108.5(5)
O(46)	Ba(07)	O(58)[8]	84.9(3)	O(29)	P(18)	O(75)	107.0(5)
O(46)	Ba(07)	O(84)[5]	87.4(3)	O(42)	P(18)	O(29)	111.0(5)

O(49)[5]	Ba(07)	O(10)[8]	76.8(2)	O(42)	P(18)	O(50)	114.0(5)
O(49)[5]	Ba(07)	O(19)[5]	76.7(2)	O(42)	P(18)	O(75)	110.5(5)
O(49)[5]	Ba(07)	O(29)[5]	103.5(3)	O(50)	P(18)	O(29)	110.6(5)
O(49)[5]	Ba(07)	O(58)[8]	114.5(2)	O(50)	P(18)	O(75)	103.2(4)
O(49)[5]	Ba(07)	O(84)[5]	75.1(2)	O(05)	P(19)	O(10)	112.9(5)
O(58)[8]	Ba(07)	O(10)[8]	54.0(2)	O(05)	P(19)	O(17)	103.7(5)
O(58)[8]	Ba(07)	O(29)[5]	99.1(2)	O(05)	P(19)	O(58)	111.6(5)
O(58)[8]	Ba(07)	O(84)[5]	167.3(2)	O(10)	P(19)	O(17)	109.7(5)
O(03)[8]	Ba(08)	O(11)[8]	79.8(2)	O(10)	P(19)	O(58)	110.8(5)
O(03)[8]	Ba(08)	O(22)	106.3(2)	O(58)	P(19)	O(17)	107.8(5)
O(03)[8]	Ba(08)	O(30)[9]	163.6(2)	O(39)	P(20)	O(92)	110.4(5)
O(03)[8]	Ba(08)	O(40)[9]	146.8(2)	O(39)	P(20)	O(95)	110.5(5)
O(03)[8]	Ba(08)	O(61)[8]	67.3(2)	O(83)	P(20)	O(39)	112.8(5)
O(03)[8]	Ba(08)	O(71)[8]	64.4(2)	O(83)	P(20)	O(92)	106.7(5)
O(11)[8]	Ba(08)	O(22)	88.1(2)	O(83)	P(20)	O(95)	109.2(5)
O(11)[8]	Ba(08)	O(30)[9]	112.3(2)	O(95)	P(20)	O(92)	107.0(5)
O(11)[8]	Ba(08)	O(61)[8]	146.4(2)	O(59)	P(21)	O(71)	108.4(5)
O(11)[8]	Ba(08)	O(71)[8]	54.5(2)	O(59)	P(21)	O(84)	111.0(4)
O(22)	Ba(08)	O(30)[9]	64.7(2)	O(71)	P(21)	O(84)	103.1(4)
O(28)	Ba(08)	O(03)[8]	65.1(2)	O(80)	P(21)	O(59)	112.2(5)
O(28)	Ba(08)	O(11)[8]	106.1(2)	O(80)	P(21)	O(71)	111.1(5)
O(28)	Ba(08)	O(22)	49.6(2)	O(80)	P(21)	O(84)	110.6(5)
O(28)	Ba(08)	O(30)[9]	100.1(2)	O(49)	P(22)	O(32)	107.1(5)
O(28)	Ba(08)	O(40)[9]	130.7(2)	O(49)	P(22)	O(66)	112.7(5)
O(28)	Ba(08)	O(55)[8]	110.2(2)	O(49)	P(22)	O(68)	112.2(5)
O(28)	Ba(08)	O(61)[8]	66.7(2)	O(66)	P(22)	O(32)	104.3(5)
O(28)	Ba(08)	O(71)[8]	128.2(2)	O(68)	P(22)	O(32)	110.3(5)
O(40)[9]	Ba(08)	O(11)[8]	67.9(2)	O(68)	P(22)	O(66)	109.8(5)
O(40)[9]	Ba(08)	O(22)	81.1(2)	O(13)	Al(1)	O(32)	116.4(4)
O(40)[9]	Ba(08)	O(30)[9]	48.3(2)	O(13)	Al(1)	O(37)	110.0(5)
O(40)[9]	Ba(08)	O(61)[8]	142.7(2)	O(13)	Al(1)	O(89)	105.4(4)
O(40)[9]	Ba(08)	O(71)[8]	89.6(2)	O(37)	Al(1)	O(32)	112.3(4)
O(55)[8]	Ba(08)	O(03)[8]	111.0(3)	O(89)	Al(1)	O(32)	105.2(4)
O(55)[8]	Ba(08)	O(11)[8]	143.4(2)	O(89)	Al(1)	O(37)	106.7(4)
O(55)[8]	Ba(08)	O(22)	119.5(2)	O(75)	Al(2)	O(66)	110.0(4)
O(55)[8]	Ba(08)	O(30)[9]	66.2(2)	O(75)	Al(2)	O(84)	105.3(4)
O(55)[8]	Ba(08)	O(40)[9]	91.6(2)	O(75)	Al(2)	O(94)	114.8(5)
O(55)[8]	Ba(08)	O(61)[8]	52.3(2)	O(84)	Al(2)	O(66)	110.2(4)
O(55)[8]	Ba(08)	O(71)[8]	97.4(2)	O(94)	Al(2)	O(66)	108.3(5)
O(61)[8]	Ba(08)	O(22)	107.1(2)	O(94)	Al(2)	O(84)	108.2(4)

O(61)[8]	Ba(08)	O(30)[9]	101.3(2)	O(11)	Al(3)	O(71)	101.6(4)
O(61)[8]	Ba(08)	O(71)[8]	102.6(2)	O(45)	Al(3)	O(11)	111.4(4)
O(71)[8]	Ba(08)	O(22)	142.0(2)	O(45)	Al(3)	O(71)	100.4(4)
O(71)[8]	Ba(08)	O(30)[9]	131.3(2)	O(45)	Al(3)	O(79)[3]	111.3(4)
O(05)[3]	Ba(11)	O(29)[2]	89.0(2)	O(79)[3]	Al(3)	O(11)	119.2(4)
O(05)[3]	Ba(11)	O(47)[3]	141.3(2)	O(79)[3]	Al(3)	O(71)	110.8(4)
O(05)[3]	Ba(11)	O(69)	113.3(2)	O(24)	P(23)	O(23)	108.7(5)
O(10)[3]	Ba(11)	O(05)[3]	53.4(2)	O(24)	P(23)	O(81)	111.1(5)
O(10)[3]	Ba(11)	O(29)[2]	70.3(2)	O(81)	P(23)	O(23)	105.8(5)
O(10)[3]	Ba(11)	O(47)[3]	165.3(2)	O(86)	P(23)	O(23)	108.2(5)
O(10)[3]	Ba(11)	O(69)	65.1(2)	O(86)	P(23)	O(24)	112.2(5)
O(29)[2]	Ba(11)	O(47)[3]	107.1(2)	O(86)	P(23)	O(81)	110.6(5)
O(29)[2]	Ba(11)	O(69)	93.1(2)	O(20)	Al(4)	O(62)	108.1(4)
O(37)[3]	Ba(11)	O(05)[3]	69.0(2)	O(48)	Al(4)	O(20)	110.8(4)
O(37)[3]	Ba(11)	O(10)[3]	116.9(2)	O(48)	Al(4)	O(62)	112.5(4)
O(37)[3]	Ba(11)	O(29)[2]	86.8(2)	O(73)	Al(4)	O(20)	109.6(4)
O(37)[3]	Ba(11)	O(47)[3]	76.9(2)	O(73)	Al(4)	O(48)	110.3(4)
O(37)[3]	Ba(11)	O(69)	177.8(2)	O(73)	Al(4)	O(62)	105.3(4)
O(47)[3]	Ba(11)	O(69)	101.1(2)	O(26)	P(24)	O(82)	111.5(5)
O(50)[2]	Ba(11)	O(05)[3]	141.5(2)	O(26)	P(24)	O(85)	110.8(5)
O(50)[2]	Ba(11)	O(10)[3]	107.6(2)	O(26)	P(24)	O(94)	107.2(5)
O(50)[2]	Ba(11)	O(29)[2]	52.6(2)	O(82)	P(24)	O(94)	105.3(5)
O(50)[2]	Ba(11)	O(37)[3]	101.7(2)	O(85)	P(24)	O(82)	111.4(5)
O(50)[2]	Ba(11)	O(47)[3]	62.3(2)	O(85)	P(24)	O(94)	110.5(5)
O(50)[2]	Ba(11)	O(69)	76.5(2)	O(17)	Al(5)	O(76)	108.1(4)
O(60)	Ba(11)	O(05)[3]	95.7(2)	O(17)	Al(5)	O(92)	113.3(5)
O(60)	Ba(11)	O(10)[3]	84.2(3)	O(35)	Al(5)	O(17)	107.8(4)
O(60)	Ba(11)	O(29)[2]	144.0(2)	O(35)	Al(5)	O(76)	115.6(4)
O(60)	Ba(11)	O(37)[3]	128.1(2)	O(35)	Al(5)	O(92)	106.1(4)
O(60)	Ba(11)	O(47)[3]	91.2(3)	O(76)	Al(5)	O(92)	106.1(5)
O(60)	Ba(11)	O(50)[2]	116.9(2)	O(16)	Al(6)	O(57)	99.5(4)
O(60)	Ba(11)	O(69)	52.4(2)	O(23)	Al(6)	O(16)	110.9(4)
O(06)[5]	Ba(12)	O(21)	89.9(2)	O(23)	Al(6)	O(44)	119.6(4)
O(06)[5]	Ba(12)	O(33)	70.1(3)	O(23)	Al(6)	O(57)	103.3(4)
O(06)[5]	Ba(12)	O(53)[1]	95.0(2)	O(44)	Al(6)	O(16)	112.9(4)
O(06)[5]	Ba(12)	O(54)[1]	82.4(2)	O(44)	Al(6)	O(57)	108.1(4)
O(06)[5]	Ba(12)	O(83)[5]	115.6(3)	O(72)	Al(7)	O(95)	108.4(4)
O(06)[5]	Ba(12)	O(88)[5]	52.7(2)	O(88)	Al(7)	O(72)	102.3(4)
O(21)	Ba(12)	O(88)[5]	73.4(2)	O(88)	Al(7)	O(93)	112.9(4)
O(33)	Ba(12)	O(21)	52.1(2)	O(88)	Al(7)	O(95)	110.4(4)

O(33)	Ba(12)	O(88)^{5}	98.6(3)
O(53)^{1}	Ba(12)	O(21)	113.0(2)
O(53)^{1}	Ba(12)	O(33)	67.4(2)
O(53)^{1}	Ba(12)	O(88)^{5}	147.7(3)
O(54)^{1}	Ba(12)	O(21)	164.7(2)
O(54)^{1}	Ba(12)	O(33)	112.7(2)
O(54)^{1}	Ba(12)	O(53)^{1}	55.0(2)
O(54)^{1}	Ba(12)	O(83)^{5}	84.4(3)
O(54)^{1}	Ba(12)	O(88)^{5}	111.3(2)
O(56)	Ba(12)	O(06)^{5}	175.9(2)
O(56)	Ba(12)	O(21)	92.4(2)
O(56)	Ba(12)	O(33)	108.7(3)
O(56)	Ba(12)	O(53)^{1}	80.9(3)
O(56)	Ba(12)	O(54)^{1}	94.6(3)
O(56)	Ba(12)	O(83)^{5}	66.7(3)
O(56)	Ba(12)	O(88)^{5}	131.2(3)
O(83)^{5}	Ba(12)	O(21)	110.8(2)
O(83)^{5}	Ba(12)	O(33)	162.9(2)
O(83)^{5}	Ba(12)	O(53)^{1}	125.7(3)
O(83)^{5}	Ba(12)	O(88)^{5}	75.2(3)
O(05)	Ba(13)	O(72)	143.5(2)
O(05)	Ba(13)	O(95)	113.4(2)
O(17)	Ba(13)	O(05)	51.1(2)
O(17)	Ba(13)	O(72)	134.5(2)
O(17)	Ba(13)	O(95)	78.7(2)
O(31)	Ba(13)	O(05)	158.7(2)
O(31)	Ba(13)	O(17)	139.0(2)
O(31)	Ba(13)	O(51)	81.5(3)
O(31)	Ba(13)	O(72)	49.7(2)
O(31)	Ba(13)	O(95)	87.9(2)
O(51)	Ba(13)	O(05)	80.9(2)
O(51)	Ba(13)	O(17)	129.1(3)
O(51)	Ba(13)	O(72)	93.3(2)
O(51)	Ba(13)	O(95)	145.3(2)
O(52)	Ba(13)	O(05)	74.3(2)
O(52)	Ba(13)	O(17)	104.0(3)
O(52)	Ba(13)	O(31)	111.8(2)
O(52)	Ba(13)	O(51)	73.1(3)
O(52)	Ba(13)	O(70)	159.5(3)
O(52)	Ba(13)	O(72)	69.6(2)
O(93)	Al(7)	O(72)	114.6(4)
O(93)	Al(7)	O(95)	108.0(4)
O(21)	Al(8)	O(67)^{5}	108.0(4)
O(27)	Al(8)	O(21)	106.1(4)
O(27)	Al(8)	O(67)^{5}	104.8(4)
O(78)	Al(8)	O(21)	111.7(4)
O(78)	Al(8)	O(27)	112.8(4)
O(78)	Al(8)	O(67)^{5}	112.9(4)
O(14)^{13}	Ba(19)	O(32)	86.3(2)
O(14)^{13}	Ba(19)	O(52)	113.4(2)
O(18)	Ba(19)	O(19)	91.3(2)
O(18)	Ba(19)	O(32)	164.8(2)
O(18)	Ba(19)	O(52)	48.9(2)
O(32)	Ba(19)	O(19)	97.1(2)
O(51)	Ba(19)	O(03)	155.7(2)
O(51)	Ba(19)	O(04)^{13}	101.2(2)
O(51)	Ba(19)	O(14)^{13}	65.7(2)
O(51)	Ba(19)	O(18)	107.0(2)
O(51)	Ba(19)	O(19)	149.8(2)
O(51)	Ba(19)	O(32)	71.2(2)
O(51)	Ba(19)	O(52)	67.6(2)
O(51)	Ba(19)	O(61)	87.0(2)
O(52)	Ba(19)	O(19)	138.5(2)
O(52)	Ba(19)	O(32)	119.3(2)
O(61)	Ba(19)	O(03)	68.9(2)
O(61)	Ba(19)	O(04)^{13}	161.3(2)
O(61)	Ba(19)	O(14)^{13}	146.0(2)
O(61)	Ba(19)	O(18)	100.0(2)
O(61)	Ba(19)	O(19)	113.9(2)
O(61)	Ba(19)	O(32)	65.1(2)
O(61)	Ba(19)	O(52)	70.1(2)
O(01)^{9}	Ba(20)	O(39)^{9}	95.8(2)
O(01)^{9}	Ba(20)	O(43)^{9}	50.9(2)
O(01)^{9}	Ba(20)	O(47)^{13}	78.5(2)
O(01)^{9}	Ba(20)	O(77)^{9}	163.4(2)
O(01)^{9}	Ba(20)	O(93)^{9}	132.7(2)
O(01)^{9}	Ba(20)	O(96)^{9}	66.6(2)
O(09)^{13}	Ba(20)	O(01)^{9}	95.2(2)
O(09)^{13}	Ba(20)	O(39)^{9}	150.8(2)
O(09)^{13}	Ba(20)	O(43)^{9}	139.2(2)

O(52)	Ba(13)	O(95)	80.5(3)	O(09)^{13}	Ba(20)	O(47)^{13}	50.6(2)
O(63)	Ba(13)	O(05)	76.3(2)	O(09)^{13}	Ba(20)	O(77)^{9}	68.3(2)
O(63)	Ba(13)	O(17)	93.1(3)	O(09)^{13}	Ba(20)	O(93)^{9}	79.9(2)
O(63)	Ba(13)	O(31)	83.7(2)	O(09)^{13}	Ba(20)	O(96)^{9}	64.6(2)
O(63)	Ba(13)	O(51)	55.1(2)	O(39)^{9}	Ba(20)	O(47)^{13}	158.6(2)
O(63)	Ba(13)	O(52)	123.3(3)	O(39)^{9}	Ba(20)	O(96)^{9}	95.5(2)
O(63)	Ba(13)	O(70)	77.0(3)	O(43)^{9}	Ba(20)	O(39)^{9}	65.9(2)
O(63)	Ba(13)	O(72)	128.9(2)	O(43)^{9}	Ba(20)	O(47)^{13}	95.4(2)
O(63)	Ba(13)	O(95)	156.2(2)	O(43)^{9}	Ba(20)	O(96)^{9}	109.8(2)
O(70)	Ba(13)	O(05)	111.9(2)	O(50)	Ba(20)	O(01)^{9}	99.4(2)
O(70)	Ba(13)	O(17)	69.5(3)	O(50)	Ba(20)	O(09)^{13}	103.8(2)
O(70)	Ba(13)	O(31)	70.0(2)	O(50)	Ba(20)	O(39)^{9}	101.0(2)
O(70)	Ba(13)	O(51)	126.5(3)	O(50)	Ba(20)	O(43)^{9}	67.0(2)
O(70)	Ba(13)	O(72)	100.6(2)	O(50)	Ba(20)	O(47)^{13}	60.3(2)
O(70)	Ba(13)	O(95)	79.2(2)	O(50)	Ba(20)	O(77)^{9}	83.0(2)
O(95)	Ba(13)	O(72)	55.9(2)	O(50)	Ba(20)	O(93)^{9}	127.6(2)
O(09)^{10}	Ba(14)	O(26)^{10}	69.8(2)	O(50)	Ba(20)	O(96)^{9}	159.4(2)
O(09)^{10}	Ba(14)	O(66)^{10}	102.8(2)	O(77)^{9}	Ba(20)	O(39)^{9}	99.9(2)
O(09)^{10}	Ba(14)	O(77)	70.0(2)	O(77)^{9}	Ba(20)	O(43)^{9}	142.2(2)
O(09)^{10}	Ba(14)	O(89)^{10}	52.1(2)	O(77)^{9}	Ba(20)	O(47)^{13}	88.6(2)
O(26)^{10}	Ba(14)	O(66)^{10}	85.5(2)	O(77)^{9}	Ba(20)	O(96)^{9}	106.2(2)
O(26)^{10}	Ba(14)	O(77)	106.2(2)	O(93)^{9}	Ba(20)	O(39)^{9}	72.7(2)
O(26)^{10}	Ba(14)	O(89)^{10}	101.8(2)	O(93)^{9}	Ba(20)	O(43)^{9}	138.3(2)
O(55)^{10}	Ba(14)	O(09)^{10}	120.7(3)	O(93)^{9}	Ba(20)	O(47)^{13}	126.1(2)
O(55)^{10}	Ba(14)	O(26)^{10}	165.2(3)	O(93)^{9}	Ba(20)	O(77)^{9}	49.2(2)
O(55)^{10}	Ba(14)	O(66)^{10}	101.1(3)	O(93)^{9}	Ba(20)	O(96)^{9}	69.1(2)
O(55)^{10}	Ba(14)	O(77)	70.9(2)	O(96)^{9}	Ba(20)	O(47)^{13}	100.9(2)
O(55)^{10}	Ba(14)	O(89)^{10}	93.0(2)	O(24)	Ba(21)	O(39)^{8}	97.0(2)
O(59)^{10}	Ba(14)	O(09)^{10}	168.4(3)	O(24)	Ba(21)	O(56)^{13}	79.6(2)
O(59)^{10}	Ba(14)	O(26)^{10}	101.4(3)	O(24)	Ba(21)	O(82)^{11}	60.9(2)
O(59)^{10}	Ba(14)	O(55)^{10}	69.5(3)	O(42)^{11}	Ba(21)	O(24)	157.0(2)
O(59)^{10}	Ba(14)	O(66)^{10}	68.2(2)	O(42)^{11}	Ba(21)	O(34)^{13}	81.9(2)
O(59)^{10}	Ba(14)	O(77)	120.8(2)	O(42)^{11}	Ba(21)	O(39)^{8}	74.8(3)
O(59)^{10}	Ba(14)	O(89)^{10}	125.4(2)	O(42)^{11}	Ba(21)	O(56)^{13}	123.4(2)
O(77)	Ba(14)	O(66)^{10}	162.2(2)	O(42)^{11}	Ba(21)	O(82)^{11}	96.3(2)
O(77)	Ba(14)	O(89)^{10}	98.6(2)	O(42)^{11}	Ba(21)	O(83)^{8}	105.1(3)
O(87)	Ba(14)	O(09)^{10}	98.0(2)	O(56)^{13}	Ba(21)	O(39)^{8}	110.9(2)
O(87)	Ba(14)	O(26)^{10}	73.5(3)	O(56)^{13}	Ba(21)	O(82)^{11}	139.4(2)
O(87)	Ba(14)	O(55)^{10}	93.9(3)	O(82)^{11}	Ba(21)	O(39)^{8}	68.1(2)
O(87)	Ba(14)	O(59)^{10}	86.4(2)	O(83)^{8}	Ba(21)	O(24)	84.5(2)

O(87)	Ba(14)	O(66)[10]	143.1(2)
O(87)	Ba(14)	O(77)	54.7(2)
O(87)	Ba(14)	O(89)[10]	147.8(2)
O(89)[10]	Ba(14)	O(66)[10]	65.3(2)
O(08)[9]	Ba(15)	O(20)	156.9(2)
O(08)[9]	Ba(15)	O(30)[9]	54.3(2)
O(08)[9]	Ba(15)	O(64)	106.8(2)
O(08)[9]	Ba(15)	O(89)	99.8(2)
O(12)	Ba(15)	O(08)[9]	80.3(3)
O(12)	Ba(15)	O(20)	97.6(2)
O(12)	Ba(15)	O(22)	176.6(3)
O(12)	Ba(15)	O(30)[9]	100.5(2)
O(12)	Ba(15)	O(64)	69.3(2)
O(12)	Ba(15)	O(68)	110.3(2)
O(12)	Ba(15)	O(89)	49.5(2)
O(22)	Ba(15)	O(08)[9]	96.9(2)
O(22)	Ba(15)	O(20)	85.7(2)
O(22)	Ba(15)	O(30)[9]	79.4(2)
O(22)	Ba(15)	O(64)	113.6(2)
O(22)	Ba(15)	O(68)	67.4(2)
O(22)	Ba(15)	O(89)	129.6(2)
O(30)[9]	Ba(15)	O(20)	104.2(2)
O(30)[9]	Ba(15)	O(64)	68.0(2)
O(30)[9]	Ba(15)	O(89)	146.2(2)
O(64)	Ba(15)	O(20)	52.0(2)
O(64)	Ba(15)	O(89)	106.3(2)
O(68)	Ba(15)	O(08)[9]	86.5(2)
O(68)	Ba(15)	O(20)	115.4(2)
O(68)	Ba(15)	O(30)[9]	124.7(2)
O(68)	Ba(15)	O(64)	166.1(2)
O(68)	Ba(15)	O(89)	66.6(2)
O(16)	Ba(16)	O(40)	94.4(2)
O(16)	Ba(16)	O(59)[11]	159.8(2)
O(16)	Ba(16)	O(65)	51.6(2)
O(16)	Ba(16)	O(78)	83.2(2)
O(16)	Ba(16)	O(80)[11]	106.7(2)
O(16)	Ba(16)	O(81)	73.7(2)
O(16)	Ba(16)	O(86)	70.2(2)
O(16)	Ba(16)	O(87)[5]	120.7(2)
O(40)	Ba(16)	O(65)	63.9(2)

O(83)[8]	Ba(21)	O(34)[13]	96.6(2)
O(83)[8]	Ba(21)	O(39)[8]	50.5(2)
O(83)[8]	Ba(21)	O(56)[13]	60.5(2)
O(83)[8]	Ba(21)	O(82)[11]	103.9(2)
O(86)	Ba(21)	O(24)	53.0(2)
O(86)	Ba(21)	O(34)[13]	76.6(2)
O(86)	Ba(21)	O(39)[8]	149.4(2)
O(86)	Ba(21)	O(42)[11]	129.9(3)
O(86)	Ba(21)	O(56)[13]	73.0(3)
O(86)	Ba(21)	O(82)[11]	89.1(2)
O(86)	Ba(21)	O(83)[8]	121.9(3)
O(02)	Ba(22)	O(15)[5]	72.5(2)
O(02)	Ba(22)	O(25)	91.9(2)
O(02)	Ba(22)	O(45)[5]	113.6(2)
O(02)	Ba(22)	O(48)	143.2(2)
O(02)	Ba(22)	O(60)[5]	111.5(2)
O(02)	Ba(22)	O(70)	54.3(2)
O(02)	Ba(22)	O(90)[5]	66.3(2)
O(15)[5]	Ba(22)	O(25)	64.7(2)
O(15)[5]	Ba(22)	O(48)	89.7(2)
O(15)[5]	Ba(22)	O(90)[5]	82.9(2)
O(25)	Ba(22)	O(90)[5]	145.6(2)
O(45)[5]	Ba(22)	O(15)[5]	52.6(2)
O(45)[5]	Ba(22)	O(25)	95.0(2)
O(45)[5]	Ba(22)	O(48)	75.9(2)
O(45)[5]	Ba(22)	O(60)[5]	72.9(2)
O(45)[5]	Ba(22)	O(70)	164.4(2)
O(45)[5]	Ba(22)	O(90)[5]	72.3(2)
O(48)	Ba(22)	O(25)	51.4(2)
O(48)	Ba(22)	O(90)[5]	144.7(2)
O(60)[5]	Ba(22)	O(15)[5]	117.8(2)
O(60)[5]	Ba(22)	O(25)	156.4(2)
O(60)[5]	Ba(22)	O(48)	105.3(2)
O(60)[5]	Ba(22)	O(70)	119.1(3)
O(60)[5]	Ba(22)	O(90)[5]	50.8(2)
O(63)	Ba(22)	O(02)	123.8(2)
O(63)	Ba(22)	O(15)[5]	159.5(2)
O(63)	Ba(22)	O(25)	99.9(2)
O(63)	Ba(22)	O(45)[5]	119.7(2)
O(63)	Ba(22)	O(48)	69.8(2)

O(40)	Ba(16)	O(86)	144.8(2)	O(63)	Ba(22)	O(60)^{5}	70.6(2)
O(40)	Ba(16)	O(87)^{5}	101.4(2)	O(63)	Ba(22)	O(70)	75.2(2)
O(59)^{11}	Ba(16)	O(40)	80.4(2)	O(63)	Ba(22)	O(90)^{5}	114.2(2)
O(59)^{11}	Ba(16)	O(65)	109.5(2)	O(70)	Ba(22)	O(15)^{5}	111.9(2)
O(59)^{11}	Ba(16)	O(78)	107.6(3)	O(70)	Ba(22)	O(25)	77.0(2)
O(59)^{11}	Ba(16)	O(80)^{11}	54.1(2)	O(70)	Ba(22)	O(48)	107.9(2)
O(59)^{11}	Ba(16)	O(81)	118.0(3)	O(70)	Ba(22)	O(90)^{5}	106.8(2)
O(59)^{11}	Ba(16)	O(86)	103.0(3)	O(04)^{8}	Ba(23)	O(76)^{8}	48.8(2)
O(59)^{11}	Ba(16)	O(87)^{5}	79.5(2)	O(04)^{8}	Ba(23)	O(92)^{8}	86.9(2)
O(65)	Ba(16)	O(86)	82.5(2)	O(15)^{5}	Ba(23)	O(04)^{8}	85.5(2)
O(65)	Ba(16)	O(87)^{5}	159.9(2)	O(15)^{5}	Ba(23)	O(25)	64.5(2)
O(78)	Ba(16)	O(40)	50.9(2)	O(15)^{5}	Ba(23)	O(76)^{8}	120.8(2)
O(78)	Ba(16)	O(65)	94.4(2)	O(15)^{5}	Ba(23)	O(92)^{8}	172.4(2)
O(78)	Ba(16)	O(86)	148.5(2)	O(19)^{5}	Ba(23)	O(04)^{8}	69.6(2)
O(78)	Ba(16)	O(87)^{5}	65.5(2)	O(19)^{5}	Ba(23)	O(15)^{5}	54.0(2)
O(80)^{11}	Ba(16)	O(40)	89.7(2)	O(19)^{5}	Ba(23)	O(25)	105.1(2)
O(80)^{11}	Ba(16)	O(65)	66.5(2)	O(19)^{5}	Ba(23)	O(76)^{8}	73.5(2)
O(80)^{11}	Ba(16)	O(78)	140.4(2)	O(19)^{5}	Ba(23)	O(92)^{8}	122.7(2)
O(80)^{11}	Ba(16)	O(86)	66.4(2)	O(24)	Ba(23)	O(04)^{8}	77.8(2)
O(80)^{11}	Ba(16)	O(87)^{5}	129.8(2)	O(24)	Ba(23)	O(15)^{5}	96.7(2)
O(81)	Ba(16)	O(40)	155.0(2)	O(24)	Ba(23)	O(19)^{5}	136.7(2)
O(81)	Ba(16)	O(65)	118.9(2)	O(24)	Ba(23)	O(25)	84.2(2)
O(81)	Ba(16)	O(78)	105.0(2)	O(24)	Ba(23)	O(54)	111.5(3)
O(81)	Ba(16)	O(80)^{11}	114.6(2)	O(24)	Ba(23)	O(76)^{8}	105.5(2)
O(81)	Ba(16)	O(86)	52.1(2)	O(24)	Ba(23)	O(92)^{8}	81.9(2)
O(81)	Ba(16)	O(87)^{5}	68.4(2)	O(25)	Ba(23)	O(04)^{8}	142.9(2)
O(86)	Ba(16)	O(87)^{5}	113.7(2)	O(25)	Ba(23)	O(76)^{8}	167.6(2)
O(07)^{12}	Ba(17)	O(01)^{6}	61.4(2)	O(06)	Ba(18)	O(52)	51.5(2)
O(07)^{12}	Ba(17)	O(12)^{3}	64.1(2)	O(06)	Ba(18)	O(54)^{2}	70.7(2)
O(07)^{12}	Ba(17)	O(34)^{12}	54.7(2)	O(06)	Ba(18)	O(61)	97.3(2)
O(07)^{12}	Ba(17)	O(47)^{3}	96.0(2)	O(06)	Ba(18)	O(73)^{2}	78.2(2)
O(07)^{12}	Ba(17)	O(64)^{3}	101.3(2)	O(28)^{2}	Ba(18)	O(54)^{2}	109.3(2)
O(07)^{12}	Ba(17)	O(65)^{6}	112.3(2)	O(38)	Ba(18)	O(05)	69.6(2)
O(07)^{12}	Ba(17)	O(79)^{3}	150.3(2)	O(38)	Ba(18)	O(06)	147.5(2)
O(12)^{3}	Ba(17)	O(01)^{6}	98.2(2)	O(38)	Ba(18)	O(28)^{2}	89.3(2)
O(12)^{3}	Ba(17)	O(47)^{3}	51.5(2)	O(38)	Ba(18)	O(52)	117.7(2)
O(12)^{3}	Ba(17)	O(64)^{3}	65.2(2)	O(38)	Ba(18)	O(54)^{2}	139.1(2)
O(12)^{3}	Ba(17)	O(79)^{3}	93.8(2)	O(38)	Ba(18)	O(58)	91.4(2)
O(34)^{12}	Ba(17)	O(01)^{6}	105.2(2)	O(38)	Ba(18)	O(61)	53.0(2)
O(34)^{12}	Ba(17)	O(12)^{3}	86.3(2)	O(38)	Ba(18)	O(73)^{2}	98.1(2)

O(34)[12]	Ba(17)	O(47)[3]	137.4(2)	O(52)	Ba(18)	O(05)	70.2(2)
O(34)[12]	Ba(17)	O(64)[3]	66.1(2)	O(52)	Ba(18)	O(28)[2]	92.1(2)
O(34)[12]	Ba(17)	O(79)[3]	107.2(2)	O(52)	Ba(18)	O(54)[2]	98.3(2)
O(47)[3]	Ba(17)	O(01)[6]	79.7(2)	O(58)	Ba(18)	O(05)	52.1(2)
O(64)[3]	Ba(17)	O(01)[6]	161.0(2)	O(58)	Ba(18)	O(06)	119.3(2)
O(64)[3]	Ba(17)	O(47)[3]	95.3(2)	O(58)	Ba(18)	O(28)[2]	166.6(2)
O(64)[3]	Ba(17)	O(79)[3]	49.5(2)	O(58)	Ba(18)	O(52)	99.3(2)
O(65)[6]	Ba(17)	O(01)[6]	51.6(2)	O(58)	Ba(18)	O(54)[2]	62.4(2)
O(65)[6]	Ba(17)	O(12)[3]	130.5(2)	O(58)	Ba(18)	O(61)	125.4(2)
O(65)[6]	Ba(17)	O(34)[12]	134.5(2)	O(58)	Ba(18)	O(73)[2]	116.6(2)
O(65)[6]	Ba(17)	O(47)[3]	82.2(2)	O(61)	Ba(18)	O(05)	75.3(2)
O(65)[6]	Ba(17)	O(64)[3]	146.4(2)	O(61)	Ba(18)	O(28)[2]	64.8(2)
O(65)[6]	Ba(17)	O(79)[3]	97.1(2)	O(61)	Ba(18)	O(52)	72.0(2)
O(79)[3]	Ba(17)	O(01)[6]	146.0(2)	O(61)	Ba(18)	O(54)[2]	167.8(2)
O(79)[3]	Ba(17)	O(47)[3]	83.3(2)	O(61)	Ba(18)	O(73)[2]	109.1(2)
O(80)	Ba(17)	O(01)[6]	106.9(2)	O(73)[2]	Ba(18)	O(05)	161.3(2)
O(80)	Ba(17)	O(07)[12]	128.2(2)	O(73)[2]	Ba(18)	O(28)[2]	50.1(2)
O(80)	Ba(17)	O(12)[3]	154.9(2)	O(73)[2]	Ba(18)	O(52)	128.4(2)
O(80)	Ba(17)	O(34)[12]	86.5(2)	O(73)[2]	Ba(18)	O(54)[2]	70.8(2)
O(80)	Ba(17)	O(47)[3]	133.4(3)	O(03)	Ba(19)	O(04)[13]	101.4(2)
O(80)	Ba(17)	O(64)[3]	89.9(2)	O(03)	Ba(19)	O(14)[13]	137.3(2)
O(80)	Ba(17)	O(65)[6]	69.1(2)	O(03)	Ba(19)	O(18)	76.6(2)
O(80)	Ba(17)	O(79)[3]	65.6(2)	O(03)	Ba(19)	O(19)	51.0(2)
O(05)	Ba(18)	O(28)[2]	139.8(2)	O(03)	Ba(19)	O(32)	99.0(2)
O(05)	Ba(18)	O(54)[2]	108.8(2)	O(03)	Ba(19)	O(52)	100.8(2)
O(06)	Ba(18)	O(05)	119.9(2)	O(04)[13]	Ba(19)	O(14)[13]	51.2(2)
O(06)	Ba(18)	O(28)[2]	63.3(2)	O(04)[13]	Ba(19)	O(18)	61.7(2)
O(04)[13]	Ba(19)	O(52)	97.3(2)	O(04)[13]	Ba(19)	O(19)	66.1(2)
O(14)[13]	Ba(19)	O(18)	106.9(2)	O(04)[13]	Ba(19)	O(32)	133.4(2)
O(14)[13]	Ba(19)	O(19)	86.3(2)				

[1]-1+X,+Y,+Z; [2]+X,1+Y,+Z; [3]1+X,1+Y,+Z; [4]-1+X,+Y,-1+Z; [5]-1+X,-1+Y,+Z; [6]1+X,1+Y,1+Z; [7]-1+X,-2+Y,+Z; [8]+X,-1+Y,+Z; [9]1+X,+Y,1+Z; [10]+X,+Y,-1+Z; [11]-1+X,-1+Y,-1+Z; [12]2+X,1+Y,1+Z; [13]1+X,+Y,+Z; [14]+X,-1+Y,-1+Z; [15]+X,+Y,1+Z; [16]+X,1+Y,1+Z; [17]-2+X,-1+Y,-1+Z

References

[1] a) G. Sheldrick, *Acta Crystallogr., Sect. A: Found. Adv.* 2015, ***71***, 3-8; b) G. Sheldrick, *Acta Crystallogr, Sect. C: Struct. Chem.* 2015, ***71***, 3-8.

[2] A. Spek, *J. Appl. Crystallogr.* 2003, ***36***, 7-13.

[3] a) M. D. Segall, P. J. D. Lindan, M. J. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark, M. C. Payne, *J. Phys.: Condens. Matter.* 2002, ***14***, 2717-2744; b) V. Milman, B. Winkler, J. A. White, C. J. Pickard, M. C. Payne, E. V. Akhmatskaya, R. H. Nobes, *Int. J. Quantum Chem.* 2000, ***77***, 895-910.

[4] J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* 1996, ***77***, 3865-3868.

[5] J. S. Lin, A. Qteish, M. C. Payne, V. Heine, *Phys. Rev. B* 1993, ***47***, 4174-4180.

[6] B. Zhang, M.-H. Lee, Z. Yang, Q. Jing, S. Pan, M. Zhang, H. Wu, X. Su, C.-S. Li, *Appl. Phys. Lett.* 2015, ***106***, 031906.

[7] J. Lin, M.-H. Lee, Z.-P. Liu, C. Chen, C. J. Pickard, *Phys. Rev. B* 1999, ***60***, 13380-13389.