Electronic Supplementary Information

Expanding the Synthetic Toolbox to Access Pristine and Rare-Earth-Doped BaFBr Nanocrystals

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1. Single Crystal X-ray Diffraction of $Ba_5(CF_2BrCOO)_{10}(H_2O)_7$

Table S1. Crystal and Structural Determination Data

Chemical formula	$Ba_5(CF_2BrCOO)_{10}(H_2O)_7$
Formula weight (g)	2538.00
Temperature (K)	100
Wavelength (Å)	0.71073
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
a, b, c (Å)	13.7278 (5), 19.6616 (9), 21.5689 (8)
α, β, γ (°)	90, 90, 90
Volume (Å^3)	5821.7 (4)
Z	4
μ (mm^{-1})	10.333
Crystal size (mm)	0.301 × 0.444 × 0.574
T_{min}, T_{max}	0.523, 0.746
θ range (º)	1.4–29.6
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.694
Index ranges	$-19 \le h \le 19$ $-27 \le k \le 27$ $-29 \le l \le 29$
Measured, independent, and observed [$I > 2\sigma(I)$] reflections	93468, 16318, 14192
Refinement method	Full−matrix least squares on F^2
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 20.1838P]$ where $P = (F_o^2 + 2F_c^2)/3$
Reflections, parameters, restraints	16318, 863, 800
H atom treatment	n/a
Δ_{max}, Δ_{min} (e Å^{-3})	1.54,–1.62
$R[F^2 > 2\sigma(F^2)]$	3.8%
$wR(F^2)$	7.9%
S	1.05

Table S2. Fractional Atomic Coordinates and Isotropic or Equivalent Displacement Parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ba1	0.52529 (4)	0.11331 (3)	0.53292 (2)	0.01180 (11)	
Ba2	0.28616 (4)	0.27560 (3)	0.56228 (2)	0.01148 (11)	
Ba3	0.23000 (4)	0.24806 (3)	0.75057 (2)	0.01054 (10)	
Ba4	0.23414 (3)	0.21123 (3)	0.94488 (2)	0.00949 (10)	
Ba5	−0.04963 (4)	0.11291 (3)	1.00466 (3)	0.01193 (11)	
C1A	0.2667 (6)	0.3780 (5)	0.8627 (4)	0.0137 (18)	
F1A	0.2024 (4)	0.3967 (3)	0.7611 (3)	0.0248 (14)	
Br1A	0.14498 (8)	0.49240 (6)	0.84262 (6)	0.0270 (3)	
O1A	0.2267 (4)	0.3211 (3)	0.8602 (3)	0.0125 (13)	
C2A	0.2400 (7)	0.4280 (5)	0.8115 (4)	0.0163 (19)	
F2A	0.3167 (4)	0.4640 (3)	0.7914 (3)	0.0258 (14)	
O2A	0.3265 (5)	0.4002 (4)	0.9011 (3)	0.0189 (15)	
F1B	0.5419 (5)	0.4130 (4)	0.7363 (4)	0.0420 (19)	
O1B	0.4105 (5)	0.3210 (4)	0.7718 (3)	0.0165 (15)	
C1B	0.4263 (6)	0.3256 (5)	0.7158 (4)	0.0137 (19)	
Br1B	0.62976 (9)	0.30099 (9)	0.69669 (8)	0.0496 (4)	
O2B	0.3747 (5)	0.3056 (4)	0.6720 (3)	0.0187 (15)	
C2B	0.5204 (8)	0.3629 (6)	0.6962 (5)	0.023 (2)	
F2B	0.5153 (5)	0.3898 (5)	0.6410 (3)	0.046 (2)	
Br1C	0.19762 (11)	−0.00553 (7)	0.61772 (8)	0.0484 (4)	
F1C	0.3569 (5)	0.0296 (4)	0.6799 (3)	0.0332 (16)	
O1C	0.2395 (5)	0.1753 (4)	0.6456 (3)	0.0170 (14)	
C1C	0.2871 (6)	0.1242 (5)	0.6277 (5)	0.0149 (19)	
F2C	0.2257 (5)	0.0708 (4)	0.7180 (3)	0.0360 (17)	
O2C	0.3445 (5)	0.1226 (4)	0.5828 (3)	0.0245 (17)	
C2C	0.2721 (8)	0.0595 (5)	0.6645 (5)	0.022 (2)	
O1D	0.4319 (5)	0.0048 (4)	0.4799 (3)	0.0198 (16)	
F1D	0.2830 (4)	0.0752 (3)	0.4398 (3)	0.0278 (14)	
C1D	0.2719 (7)	0.0077 (5)	0.4364 (4)	0.0137 (18)	
C2D	0.3578 (6)	−0.0296 (5)	0.4673 (4)	0.0119 (18)	
O2D	0.3467 (5)	−0.0910 (3)	0.4762 (3)	0.0170 (14)	
F2D	0.1882 (4)	−0.0083 (3)	0.4634 (3)	0.0253 (14)	
Br2D	0.26349 (9)	−0.01768 (7)	0.35057 (5)	0.0317 (3)	
O1E	0.5104 (5)	0.1687 (4)	0.4154 (3)	0.0202 (16)	

O2E	0.6380 (5)	0.1930 (4)	0.3544 (3)	0.0168 (15)	
C1E	0.5529 (7)	0.1768 (5)	0.3657 (4)	0.0151 (16)	
C2E	0.4886 (7)	0.1637 (6)	0.3088 (5)	0.0192 (13)	0.917 (4)
F1E	0.3995 (5)	0.1890 (5)	0.3175 (3)	0.0271 (16)	0.917 (4)
F2E	0.5254 (4)	0.1936 (3)	0.2576 (3)	0.0198 (12)	0.917 (4)
Br1E	0.47877 (12)	0.06873 (8)	0.29285 (8)	0.0413 (5)	0.917 (4)
C3E	0.5063 (16)	0.1370 (15)	0.3116 (12)	0.0192 (13)	0.083 (4)
F3E	0.515 (3)	0.0698 (14)	0.322 (3)	0.021 (4)	0.083 (4)
F4E	0.553 (2)	0.152 (3)	0.2577 (12)	0.020 (2)	0.083 (4)
Br2E	0.3722 (10)	0.1586 (10)	0.2985 (7)	0.032 (3)	0.083 (4)
O1F	0.4742 (4)	0.2502 (4)	0.5366 (3)	0.0147 (13)	
O2F	0.6289 (5)	0.2614 (4)	0.5055 (3)	0.0246 (18)	
C1F	0.5443 (6)	0.2815 (5)	0.5130 (4)	0.0147 (17)	
C2F	0.5153 (9)	0.3531 (6)	0.4887 (5)	0.023 (2)	0.869 (11)
F1F	0.5844 (6)	0.3986 (4)	0.5034 (4)	0.038 (2)	0.869 (11)
F2F	0.4336 (6)	0.3751 (4)	0.5152 (3)	0.031 (2)	0.869 (11)
Br1F	0.4963 (2)	0.35186 (18)	0.40093 (9)	0.0210 (5)	0.869 (11)
C3F	0.546 (2)	0.3547 (9)	0.4869 (12)	0.023 (2)	0.131 (11)
F3F	0.637 (2)	0.3751 (19)	0.4775 (19)	0.030 (7)	0.131 (11)
F4F	0.504 (3)	0.3977 (14)	0.5260 (15)	0.034 (6)	0.131 (11)
Br2F	0.4724 (18)	0.3527 (12)	0.4119 (11)	0.047 (5)	0.131 (11)
O1G	0.1529 (5)	0.4971 (4)	0.5106 (3)	0.0196 (16)	
O2G	0.2073 (5)	0.3935 (4)	0.5288 (4)	0.0297 (18)	
C1G	0.2054 (7)	0.4554 (5)	0.5354 (5)	0.0182 (19)	
C2G	0.2801 (7)	0.4844 (6)	0.5830 (5)	0.0183 (18)	0.940 (4)
Br1G	0.21515 (10)	0.53397 (8)	0.64717 (6)	0.0316 (4)	0.940 (4)
F1G	0.3320 (5)	0.4347 (4)	0.6098 (3)	0.0282 (16)	0.940 (4)
F2G	0.3440 (5)	0.5256 (4)	0.5551 (3)	0.0267 (17)	0.940 (4)
C3G	0.3007 (15)	0.479 (2)	0.5674 (12)	0.0183 (18)	0.060 (4)
Br2G	0.2568 (18)	0.4979 (14)	0.6495 (8)	0.037 (6)	0.060 (4)
F3G	0.369 (3)	0.431 (4)	0.570 (3)	0.022 (5)	0.060 (4)
F4G	0.338 (5)	0.535 (4)	0.5418 (19)	0.020 (8)	0.060 (4)
O2H	0.3954 (4)	0.1635 (4)	0.7498 (3)	0.0181 (15)	
O1H	0.3407 (5)	0.1817 (4)	0.8454 (3)	0.0227 (16)	
C1H	0.4012 (7)	0.1589 (5)	0.8069 (5)	0.0180 (19)	
C2H	0.4859 (8)	0.1191 (6)	0.8342 (5)	0.021 (2)	0.894 (4)
F1H	0.5164 (7)	0.0684 (5)	0.7983 (4)	0.030 (2)	0.894 (4)

F2H	0.4671 (5)	0.0925 (4)	0.8896 (3)	0.0341 (18)	0.894 (4)
Br1H	0.59134 (9)	0.18391 (8)	0.84440 (8)	0.0366 (5)	0.894 (4)
C3H	0.5040 (14)	0.1442 (11)	0.8296 (14)	0.021 (2)	0.106 (4)
F3H	0.578 (2)	0.1716 (17)	0.799 (2)	0.025 (7)	0.106 (4)
F4H	0.521 (3)	0.1583 (19)	0.8890 (15)	0.031 (6)	0.106 (4)
Br2H	0.5091 (12)	0.0460 (7)	0.8208 (8)	0.036 (4)	0.106 (4)
C1I	−0.0134 (6)	0.2758 (5)	0.9938 (4)	0.0130 (18)	
Br1I	−0.03650 (7)	0.33861 (5)	0.87650 (5)	0.0187 (2)	
F1I	−0.0977 (4)	0.3815 (3)	0.9879 (3)	0.0243 (13)	
O1I	0.0656 (4)	0.2471 (4)	0.9912 (3)	0.0172 (14)	
F2I	0.0584 (4)	0.3847 (4)	0.9766 (3)	0.0285 (15)	
C2I	−0.0212 (7)	0.3468 (5)	0.9652 (5)	0.0154 (19)	
O3I	−0.0901 (4)	0.2532 (4)	1.0161 (3)	0.0187 (15)	
O1J	0.1150 (4)	0.1924 (4)	0.8409 (3)	0.0146 (14)	
O2J	−0.0129 (5)	0.1457 (4)	0.8885 (3)	0.0239 (17)	
C1J	0.0341 (7)	0.1631 (5)	0.8433 (4)	0.0175 (18)	
C2J	−0.0103 (7)	0.1435 (6)	0.7806 (5)	0.0234 (18)	
F1J	0.0443 (5)	0.1672 (4)	0.7329 (3)	0.0315 (15)	
F2J	−0.0129 (5)	0.0767 (4)	0.7738 (3)	0.0371 (17)	
Br1J	−0.14003 (8)	0.17768 (7)	0.76957 (6)	0.0363 (3)	
O1W	0.5338 (6)	−0.0027 (4)	0.6130 (4)	0.0292 (19)	
O2W	0.5297 (6)	0.1300 (5)	0.6613 (3)	0.031 (2)	
O3W	0.7112 (6)	0.1495 (5)	0.6084 (4)	0.045 (2)	
O4W	0.3135 (5)	0.2274 (4)	0.4401 (4)	0.0246 (17)	
O5W	0.2593 (5)	0.3346 (4)	1.0251 (3)	0.0191 (15)	
O6W	0.2236 (5)	0.2028 (4)	1.0801 (3)	0.0202 (15)	
O7W	0.0439 (6)	0.1406 (5)	1.1220 (4)	0.0331 (19)	

Table S3. Anisotropic Atomic Displacement Parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.0154 (2)	0.0083 (2)	0.0117 (2)	0.0019 (2)	0.0020 (2)	0.0003 (2)
Ba2	0.0093 (2)	0.0147 (3)	0.0104 (2)	0.00317 (19)	−0.00006 (19)	−0.0013 (2)
Ba3	0.0100 (2)	0.0124 (3)	0.0092 (2)	0.0004 (2)	−0.0003 (2)	−0.0001 (2)
Ba4	0.0072 (2)	0.0108 (3)	0.0104 (2)	−0.00055 (18)	0.00032 (19)	0.0004 (2)
Ba5	0.0130 (2)	0.0088 (3)	0.0139 (3)	−0.0006 (2)	0.0045 (2)	−0.0004 (2)
C1A	0.011 (4)	0.010 (4)	0.020 (5)	0.002 (3)	−0.003 (4)	0.002 (4)
F1A	0.033 (3)	0.021 (3)	0.021 (3)	0.002 (3)	−0.016 (3)	−0.002 (3)
Br1A	0.0290 (5)	0.0128 (5)	0.0390 (7)	0.0067 (4)	−0.0090 (5)	0.0004 (5)
O1A	0.015 (3)	0.006 (3)	0.017 (3)	−0.001 (3)	0.004 (3)	0.001 (3)
C2A	0.020 (4)	0.010 (5)	0.019 (5)	−0.003 (4)	−0.003 (4)	0.003 (4)
F2A	0.030 (3)	0.022 (4)	0.026 (3)	−0.007 (3)	−0.002 (3)	0.007 (3)
O2A	0.023 (3)	0.018 (4)	0.015 (3)	−0.001 (3)	−0.007 (3)	0.002 (3)
F1B	0.032 (4)	0.033 (4)	0.062 (5)	−0.017 (3)	0.000 (3)	−0.015 (4)
O1B	0.019 (3)	0.017 (4)	0.014 (3)	−0.004 (3)	0.001 (3)	−0.002 (3)
C1B	0.010 (4)	0.016 (5)	0.015 (5)	0.002 (3)	0.003 (3)	0.001 (4)
Br1B	0.0196 (5)	0.0511 (9)	0.0781 (11)	0.0064 (5)	0.0126 (6)	0.0125 (8)
O2B	0.015 (3)	0.030 (4)	0.012 (3)	−0.001 (3)	−0.004 (3)	0.000 (3)
C2B	0.021 (5)	0.035 (7)	0.015 (5)	−0.002 (4)	0.000 (4)	0.004 (5)
F2B	0.028 (3)	0.073 (6)	0.037 (4)	−0.016 (4)	−0.002 (3)	0.031 (4)
Br1C	0.0619 (9)	0.0191 (6)	0.0643 (10)	−0.0191 (6)	−0.0310 (8)	0.0085 (6)
F1C	0.033 (3)	0.020 (4)	0.047 (4)	0.008 (3)	−0.011 (3)	0.000 (3)
O1C	0.020 (3)	0.011 (3)	0.020 (3)	0.005 (3)	−0.003 (3)	−0.006 (3)
C1C	0.012 (4)	0.011 (5)	0.022 (5)	−0.002 (3)	−0.005 (4)	0.000 (4)
F2C	0.041 (4)	0.039 (4)	0.028 (4)	−0.002 (3)	0.009 (3)	0.018 (3)
O2C	0.016 (3)	0.034 (5)	0.023 (4)	−0.002 (3)	0.008 (3)	−0.002 (4)
C2C	0.023 (5)	0.011 (5)	0.031 (6)	−0.005 (4)	−0.001 (5)	0.007 (4)
O1D	0.020 (3)	0.009 (3)	0.030 (4)	−0.003 (3)	−0.006 (3)	−0.005 (3)
F1D	0.0285 (17)	0.0245 (18)	0.0304 (18)	0.0005 (13)	−0.0015 (13)	0.0001 (13)
C1D	0.016 (4)	0.011 (4)	0.014 (4)	0.001 (3)	0.005 (3)	0.004 (3)
C2D	0.010 (4)	0.013 (5)	0.012 (4)	0.000 (3)	0.002 (3)	0.001 (4)
O2D	0.021 (3)	0.005 (3)	0.025 (4)	−0.001 (3)	−0.003 (3)	0.002 (3)
F2D	0.019 (3)	0.032 (4)	0.025 (3)	0.005 (3)	0.005 (2)	0.006 (3)
Br2D	0.0304 (6)	0.0454 (8)	0.0194 (5)	−0.0037 (5)	−0.0058 (5)	−0.0005 (5)
O1E	0.021 (3)	0.027 (4)	0.013 (3)	−0.008 (3)	0.002 (3)	0.006 (3)
O2E	0.018 (3)	0.022 (4)	0.010 (3)	−0.008 (3)	−0.003 (3)	−0.002 (3)

C1E	0.014 (3)	0.019 (4)	0.012 (3)	−0.001 (3)	0.001 (3)	−0.001 (3)
C2E	0.016 (2)	0.025 (3)	0.017 (3)	−0.003 (2)	0.002 (2)	0.000 (3)
F1E	0.016 (3)	0.042 (5)	0.023 (4)	0.008 (3)	0.003 (3)	0.000 (3)
F2E	0.016 (2)	0.028 (3)	0.015 (3)	−0.004 (2)	0.001 (2)	0.005 (2)
Br1E	0.0519 (9)	0.0256 (8)	0.0465 (9)	−0.0222 (6)	0.0192 (7)	−0.0196 (7)
C3E	0.016 (2)	0.025 (3)	0.017 (3)	−0.003 (2)	0.002 (2)	0.000 (3)
F3E	0.021 (7)	0.022 (6)	0.021 (7)	−0.009 (6)	0.001 (7)	−0.006 (6)
F4E	0.016 (5)	0.027 (5)	0.017 (4)	−0.004 (4)	0.001 (4)	0.001 (4)
Br2E	0.025 (6)	0.043 (7)	0.029 (6)	0.002 (5)	−0.004 (5)	−0.001 (6)
O1F	0.012 (3)	0.016 (3)	0.016 (3)	0.002 (3)	0.006 (2)	0.005 (3)
O2F	0.013 (3)	0.043 (5)	0.018 (4)	0.001 (3)	0.000 (3)	−0.009 (4)
C1F	0.017 (4)	0.013 (4)	0.014 (4)	−0.001 (3)	0.002 (3)	−0.001 (3)
C2F	0.030 (4)	0.014 (4)	0.023 (4)	−0.005 (4)	0.003 (4)	0.003 (3)
F1F	0.044 (5)	0.026 (4)	0.043 (5)	−0.022 (4)	−0.017 (4)	0.008 (4)
F2F	0.046 (4)	0.014 (4)	0.032 (4)	0.011 (3)	0.018 (3)	0.004 (3)
Br1F	0.0266 (10)	0.0218 (9)	0.0146 (8)	0.0068 (8)	0.0017 (6)	0.0024 (6)
C3F	0.030 (4)	0.014 (4)	0.023 (4)	−0.005 (4)	0.003 (4)	0.003 (3)
F3F	0.031 (12)	0.024 (13)	0.036 (14)	−0.018 (11)	−0.011 (11)	0.003 (13)
F4F	0.052 (12)	0.021 (10)	0.030 (12)	0.002 (11)	0.003 (11)	−0.001 (11)
Br2F	0.044 (10)	0.015 (6)	0.081 (11)	0.011 (7)	−0.006 (8)	0.006 (8)
O1G	0.021 (3)	0.010 (4)	0.028 (4)	0.004 (3)	−0.008 (3)	0.000 (3)
O2G	0.025 (3)	0.013 (3)	0.051 (4)	−0.004 (3)	−0.010 (3)	−0.003 (3)
C1G	0.017 (4)	0.013 (4)	0.024 (5)	0.004 (3)	0.000 (4)	0.001 (4)
C2G	0.017 (4)	0.015 (4)	0.023 (4)	0.002 (3)	−0.002 (3)	0.001 (4)
Br1G	0.0353 (7)	0.0355 (9)	0.0241 (6)	0.0121 (6)	0.0033 (5)	−0.0041 (6)
F1G	0.028 (3)	0.021 (4)	0.036 (4)	0.009 (3)	−0.012 (3)	0.002 (3)
F2G	0.027 (3)	0.023 (4)	0.030 (4)	−0.011 (3)	0.006 (3)	0.003 (3)
C3G	0.017 (4)	0.015 (4)	0.023 (4)	0.002 (3)	−0.002 (3)	0.001 (4)
Br2G	0.046 (10)	0.040 (11)	0.023 (8)	0.010 (9)	−0.002 (8)	−0.004 (8)
F3G	0.022 (8)	0.018 (9)	0.025 (9)	0.002 (8)	−0.004 (9)	0.002 (9)
F4G	0.020 (14)	0.017 (12)	0.023 (16)	−0.002 (11)	−0.002 (15)	0.003 (13)
O2H	0.016 (3)	0.026 (4)	0.012 (3)	0.007 (3)	−0.003 (3)	−0.008 (3)
O1H	0.023 (4)	0.026 (4)	0.020 (4)	0.010 (3)	0.008 (3)	0.000 (3)
C1H	0.020 (4)	0.015 (5)	0.019 (5)	0.003 (4)	0.000 (4)	−0.004 (4)
C2H	0.018 (4)	0.023 (5)	0.023 (4)	0.001 (4)	0.000 (3)	−0.004 (4)
F1H	0.030 (4)	0.031 (5)	0.029 (5)	0.019 (4)	−0.007 (4)	−0.012 (4)
F2H	0.030 (4)	0.047 (5)	0.025 (4)	0.006 (3)	0.003 (3)	0.014 (3)

Br1H	0.0195 (6)	0.0325 (8)	0.0577 (11)	−0.0034 (5)	−0.0168 (6)	0.0054 (7)
C3H	0.018 (4)	0.023 (5)	0.023 (4)	0.001 (4)	0.000 (3)	−0.004 (4)
F3H	0.024 (9)	0.026 (11)	0.025 (10)	0.001 (9)	0.001 (9)	−0.007 (10)
F4H	0.028 (10)	0.034 (11)	0.029 (9)	0.000 (9)	−0.005 (8)	0.000 (9)
Br2H	0.038 (6)	0.023 (6)	0.046 (7)	0.008 (5)	−0.011 (6)	−0.002 (5)
C1I	0.011 (4)	0.015 (5)	0.013 (4)	−0.007 (3)	0.000 (3)	−0.002 (4)
Br1I	0.0207 (5)	0.0200 (5)	0.0155 (5)	0.0022 (4)	0.0027 (4)	0.0024 (4)
F1I	0.033 (3)	0.015 (3)	0.025 (3)	0.012 (2)	0.002 (2)	−0.003 (3)
O1I	0.012 (3)	0.021 (4)	0.019 (3)	0.003 (3)	0.003 (3)	0.002 (3)
F2I	0.029 (3)	0.024 (3)	0.032 (3)	−0.014 (3)	−0.009 (3)	0.004 (3)
C2I	0.015 (4)	0.010 (5)	0.021 (5)	0.000 (4)	0.004 (4)	0.000 (4)
O3I	0.007 (3)	0.018 (4)	0.031 (4)	−0.001 (3)	0.004 (3)	−0.002 (3)
O1J	0.015 (3)	0.016 (4)	0.014 (3)	−0.002 (3)	−0.004 (3)	0.000 (3)
O2J	0.027 (4)	0.029 (5)	0.016 (4)	−0.008 (3)	0.001 (3)	0.002 (3)
C1J	0.019 (4)	0.021 (4)	0.013 (4)	−0.004 (4)	−0.003 (3)	−0.001 (4)
C2J	0.023 (3)	0.032 (4)	0.016 (3)	−0.006 (3)	−0.004 (3)	−0.002 (3)
F1J	0.033 (3)	0.050 (4)	0.012 (3)	−0.012 (3)	0.000 (2)	−0.004 (3)
F2J	0.039 (4)	0.027 (4)	0.046 (4)	−0.007 (3)	−0.009 (3)	−0.014 (3)
Br1J	0.0209 (5)	0.0429 (8)	0.0450 (7)	−0.0099 (5)	−0.0140 (5)	0.0174 (6)
O1W	0.042 (5)	0.022 (4)	0.024 (4)	0.018 (4)	0.001 (4)	0.005 (3)
O2W	0.027 (4)	0.043 (6)	0.022 (4)	0.004 (4)	0.000 (3)	−0.011 (4)
O3W	0.033 (5)	0.053 (7)	0.050 (6)	0.001 (4)	0.001 (4)	0.003 (5)
O4W	0.022 (3)	0.028 (4)	0.024 (4)	−0.002 (3)	0.007 (3)	−0.007 (4)
O5W	0.017 (3)	0.019 (4)	0.021 (3)	−0.003 (3)	0.005 (3)	−0.006 (3)
O6W	0.018 (3)	0.025 (4)	0.018 (3)	−0.002 (3)	0.002 (3)	0.002 (3)
O7W	0.033 (2)	0.034 (2)	0.032 (2)	−0.0011 (13)	0.0004 (13)	0.0001 (13)

Table S4. Geometric Parameters (Å, º)

Ba1—O2C	2.711 (6)	C1B—C2B	1.545 (14)
Ba1—O1D	2.740 (7)	Br1B—C2B	1.932 (11)
Ba1—O1E	2.767 (7)	C2B—F2B	1.306 (12)
Ba1—O1F	2.783 (7)	Br1C—C2C	1.924 (11)
Ba1—O2W	2.790 (7)	F1C—C2C	1.347 (12)
Ba1—O2G^{i}	2.834 (7)	O1C—C1C	1.258 (11)
Ba1—O1W	2.864 (8)	C1C—O2C	1.250 (11)
Ba1—O1G^{i}	2.943 (7)	C1C—C2C	1.513 (14)
Ba1—O3W	3.110 (9)	F2C—C2C	1.337 (12)
Ba1—C1G^{i}	3.180 (10)	O1D—C2D	1.251 (11)
Ba1—O2F	3.293 (8)	F1D—C1D	1.338 (11)
Ba1—C1F	3.344 (10)	C1D—F2D	1.326 (10)
Ba2—O2G	2.658 (8)	C1D—C2D	1.540 (13)
Ba2—O1F	2.687 (6)	C1D—Br2D	1.921 (10)
Ba2—O2F^{ii}	2.707 (7)	C2D—O2D	1.233 (11)
Ba2—O2B	2.726 (6)	O1E—C1E	1.230 (11)
Ba2—O1C	2.744 (7)	O2E—C1E	1.235 (11)
Ba2—O2E^{ii}	2.784 (6)	C1E—C2E	1.533 (14)
Ba2—O4W	2.826 (7)	C1E—C3E	1.543 (18)
Ba2—F2F	2.993 (8)	C2E—F1E	1.334 (12)
Ba2—O2C	3.145 (8)	C2E—F2E	1.349 (12)
Ba2—F3G	3.27 (8)	C2E—Br1E	1.904 (12)
Ba2—C1C	3.294 (10)	C3E—F3E	1.343 (18)
Ba2—Ba3	4.1690 (8)	C3E—F4E	1.356 (18)
Ba3—O1C	2.682 (7)	C3E—Br2E	1.910 (17)
Ba3—O1J	2.735 (7)	O1F—C1F	1.249 (11)
Ba3—O1A	2.767 (6)	O2F—C1F	1.238 (11)
Ba3—O2H	2.814 (6)	C1F—C3F	1.547 (19)
Ba3—O2E^{ii}	2.839 (7)	C1F—C2F	1.555 (15)
Ba3—O2B	2.845 (7)	C2F—F2F	1.330 (14)
Ba3—O1H	2.864 (7)	C2F—F1F	1.341 (14)
Ba3—O1B	2.899 (7)	C2F—Br1F	1.912 (12)
Ba3—F1A	2.957 (6)	C3F—F4F	1.325 (19)
Ba3—F1J	3.028 (6)	C3F—F3F	1.335 (19)
Ba3—F2E^{ii}	3.038 (6)	C3F—Br2F	1.905 (17)
Ba3—F4E^{ii}	3.14 (4)	O1G—C1G	1.215 (12)

Ba4—O1I	2.617 (6)	O2G—C1G	1.227 (12)
Ba4—O3I^{iii}	2.650 (6)	C1G—C3G	1.550 (19)
Ba4—O1H	2.661 (7)	C1G—C2G	1.559 (14)
Ba4—O2D^{iv}	2.697 (7)	C2G—F2G	1.337 (12)
Ba4—O1J	2.801 (6)	C2G—F1G	1.340 (12)
Ba4—O1A	2.830 (6)	C2G—Br1G	1.914 (11)
Ba4—O6W	2.924 (7)	C3G—F4G	1.328 (18)
Ba4—O5W	2.999 (7)	C3G—F3G	1.332 (18)
Ba4—F1I^{iii}	3.279 (7)	C3G—Br2G	1.907 (18)
Ba4—Ba5	4.5360 (7)	O2H—C1H	1.237 (12)
Ba4—Ba5^{iii}	4.6852 (8)	O1H—C1H	1.256 (12)
Ba5—O2J	2.636 (7)	C1H—C2H	1.520 (15)
Ba5—O2A^{v}	2.663 (6)	C1H—C3H	1.522 (19)
Ba5—O1G^{vi}	2.702 (7)	C2H—F2H	1.330 (13)
Ba5—O3I	2.824 (8)	C2H—F1H	1.331 (14)
Ba5—O1D^{iv}	2.873 (7)	C2H—Br1H	1.941 (12)
Ba5—O2D^{iv}	2.885 (6)	C3H—F3H	1.330 (19)
Ba5—O7W	2.890 (8)	C3H—F4H	1.332 (18)
Ba5—O5W^{v}	2.892 (6)	C3H—Br2H	1.943 (18)
Ba5—O1I	3.089 (7)	C1I—O1I	1.223 (11)
Ba5—O1W^{iv}	3.194 (8)	C1I—O3I	1.240 (10)
Ba5—C2D^{iv}	3.204 (9)	C1I—C2I	1.530 (14)
Ba5—C1I	3.249 (10)	Br1I—C2I	1.930 (10)
C1A—O2A	1.245 (11)	F1I—C2I	1.345 (11)
C1A—O1A	1.247 (11)	F2I—C2I	1.346 (11)
C1A—C2A	1.524 (13)	O1J—C1J	1.252 (11)
F1A—C2A	1.351 (11)	O2J—C1J	1.218 (12)
Br1A—C2A	1.937 (10)	C1J—C2J	1.533 (14)
C2A—F2A	1.342 (11)	C2J—F2J	1.322 (14)
F1B—C2B	1.343 (13)	C2J—F1J	1.356 (12)
O1B—C1B	1.229 (11)	C2J—Br1J	1.918 (11)
C1B—O2B	1.244 (11)		
O2C—Ba1—O1D	77.9 (2)	O2J—Ba5—O3I	83.2 (2)
O2C—Ba1—O1E	105.7 (2)	O2A^{v}—Ba5—O3I	84.4 (2)
O1D—Ba1—O1E	83.6 (2)	O1G^{vi}—Ba5—O3I	136.92 (19)
O2C—Ba1—O1F	72.1 (2)	O2J—Ba5—O1D^{iv}	85.0 (2)

O1D—Ba1—O1F	130.4 (2)	O2A^{v}—Ba5—O1D^{iv}	115.0 (2)
O1E—Ba1—O1F	68.1 (2)	O1G^{vi}—Ba5—O1D^{iv}	66.0 (2)
O2C—Ba1—O2W	67.5 (2)	O3I—Ba5—O1D^{iv}	155.98 (18)
O1D—Ba1—O2W	121.1 (2)	O2J—Ba5—O2D^{iv}	69.5 (2)
O1E—Ba1—O2W	149.9 (2)	O2A^{v}—Ba5—O2D^{iv}	139.8 (2)
O1F—Ba1—O2W	82.2 (2)	O1G^{vi}—Ba5—O2D^{iv}	110.8 (2)
O2C—Ba1—O2G^{i}	175.3 (2)	O3I—Ba5—O2D^{iv}	110.73 (18)
O1D—Ba1—O2G^{i}	100.4 (2)	O1D^{iv}—Ba5—O2D^{iv}	45.33 (18)
O1E—Ba1—O2G^{i}	69.7 (2)	O2J—Ba5—O7W	134.5 (2)
O1F—Ba1—O2G^{i}	106.3 (2)	O2A^{v}—Ba5—O7W	68.5 (2)
O2W—Ba1—O2G^{i}	116.9 (2)	O1G^{vi}—Ba5—O7W	119.9 (2)
O2C—Ba1—O1W	81.5 (2)	O3I—Ba5—O7W	80.0 (2)
O1D—Ba1—O1W	69.5 (2)	O1D^{iv}—Ba5—O7W	93.7 (2)
O1E—Ba1—O1W	150.3 (2)	O2D^{iv}—Ba5—O7W	77.6 (2)
O1F—Ba1—O1W	139.8 (2)	O2J—Ba5—O5W^{v}	82.8 (2)
O2W—Ba1—O1W	59.6 (2)	O2A^{v}—Ba5—O5W^{v}	68.0 (2)
O2G^{i}—Ba1—O1W	102.1 (2)	O1G^{vi}—Ba5—O5W^{v}	78.3 (2)
O2C—Ba1—O1G^{i}	136.1 (2)	O3I—Ba5—O5W^{v}	59.49 (19)
O1D—Ba1—O1G^{i}	64.58 (19)	O1D^{iv}—Ba5—O5W^{v}	139.2 (2)
O1E—Ba1—O1G^{i}	92.4 (2)	O2D^{iv}—Ba5—O5W^{v}	151.9 (2)
O1F—Ba1—O1G^{i}	150.76 (18)	O7W—Ba5—O5W^{v}	122.0 (2)
O2W—Ba1—O1G^{i}	113.0 (2)	O2J—Ba5—O1I	66.6 (2)
O2G^{i}—Ba1—O1G^{i}	44.8 (2)	O2A^{v}—Ba5—O1I	118.8 (2)
O1W—Ba1—O1G^{i}	65.2 (2)	O1G^{vi}—Ba5—O1I	167.6 (2)
O2C—Ba1—O3W	121.9 (2)	O3I—Ba5—O1I	43.53 (17)
O1D—Ba1—O3W	141.4 (2)	O1D^{iv}—Ba5—O1I	112.47 (18)
O1E—Ba1—O3W	116.8 (2)	O2D^{iv}—Ba5—O1I	67.23 (18)
O1F—Ba1—O3W	88.3 (2)	O7W—Ba5—O1I	72.2 (2)
O2W—Ba1—O3W	55.6 (2)	O5W^{v}—Ba5—O1I	97.97 (19)
O2G^{i}—Ba1—O3W	62.2 (2)	O2J—Ba5—O1W^{iv}	148.1 (2)
O1W—Ba1—O3W	80.4 (3)	O2A^{v}—Ba5—O1W^{iv}	54.5 (2)
O1G^{i}—Ba1—O3W	81.2 (2)	O1G^{vi}—Ba5—O1W^{iv}	63.5 (2)
O2C—Ba1—C1G^{i}	157.6 (3)	O3I—Ba5—O1W^{iv}	127.7 (2)
O1D—Ba1—C1G^{i}	80.7 (2)	O1D^{iv}—Ba5—O1W^{iv}	63.4 (2)
O1E—Ba1—C1G^{i}	78.5 (2)	O2D^{iv}—Ba5—O1W^{iv}	89.4 (2)
O1F—Ba1—C1G^{i}	128.3 (2)	O7W—Ba5—O1W^{iv}	57.1 (2)
O2W—Ba1—C1G^{i}	119.5 (2)	O5W^{v}—Ba5—O1W^{iv}	117.8 (2)

O2G^{i}—Ba1—C1G^{i}	22.6 (2)	O1I—Ba5—O1W^{iv}	127.82 (19)
O1W—Ba1—C1G^{i}	84.8 (2)	O2J—Ba5—C2D^{iv}	74.3 (2)
O1G^{i}—Ba1—C1G^{i}	22.5 (2)	O2A^{v}—Ba5—C2D^{iv}	131.9 (2)
O3W—Ba1—C1G^{i}	72.7 (3)	O1G^{vi}—Ba5—C2D^{iv}	88.3 (2)
O2C—Ba1—O2F	114.0 (2)	O3I—Ba5—C2D^{iv}	133.1 (2)
O1D—Ba1—O2F	144.7 (2)	O1D^{iv}—Ba5—C2D^{iv}	22.9 (2)
O1E—Ba1—O2F	61.31 (19)	O2D^{iv}—Ba5—C2D^{iv}	22.6 (2)
O1F—Ba1—O2F	42.18 (17)	O7W—Ba5—C2D^{iv}	87.2 (2)
O2W—Ba1—O2F	93.7 (2)	O5W^{v}—Ba5—C2D^{iv}	150.7 (2)
O2G^{i}—Ba1—O2F	64.9 (2)	O1I—Ba5—C2D^{iv}	89.5 (2)
O1W—Ba1—O2F	142.6 (2)	O1W^{iv}—Ba5—C2D^{iv}	77.4 (2)
O1G^{i}—Ba1—O2F	109.74 (18)	O2J—Ba5—C1I	70.1 (2)
O3W—Ba1—O2F	62.4 (2)	O2A^{v}—Ba5—C1I	104.4 (2)
C1G^{i}—Ba1—O2F	87.5 (2)	O1G^{vi}—Ba5—C1I	154.4 (2)
O2C—Ba1—C1F	93.2 (2)	O3I—Ba5—C1I	22.17 (19)
O1D—Ba1—C1F	138.8 (2)	O1D^{iv}—Ba5—C1I	134.0 (2)
O1E—Ba1—C1F	60.0 (2)	O2D^{iv}—Ba5—C1I	89.1 (2)
O1F—Ba1—C1F	21.09 (19)	O7W—Ba5—C1I	79.0 (2)
O2W—Ba1—C1F	90.6 (2)	O5W^{v}—Ba5—C1I	76.8 (2)
O2G^{i}—Ba1—C1F	85.3 (2)	O1I—Ba5—C1I	22.07 (19)
O1W—Ba1—C1F	149.5 (2)	O1W^{iv}—Ba5—C1I	135.3 (2)
O1G^{i}—Ba1—C1F	129.9 (2)	C2D^{iv}—Ba5—C1I	111.1 (2)
O3W—Ba1—C1F	77.1 (2)	O2A—C1A—O1A	129.4 (9)
C1G^{i}—Ba1—C1F	107.5 (2)	O2A—C1A—C2A	114.4 (8)
O2F—Ba1—C1F	21.48 (19)	O1A—C1A—C2A	116.2 (8)
O2G—Ba2—O1F	119.8 (2)	C2A—F1A—Ba3	117.6 (5)
O2G—Ba2—O2F^{ii}	76.3 (2)	C1A—O1A—Ba3	119.7 (6)
O1F—Ba2—O2F^{ii}	127.2 (2)	C1A—O1A—Ba4	129.8 (6)
O2G—Ba2—O2B	103.2 (2)	Ba3—O1A—Ba4	98.9 (2)
O1F—Ba2—O2B	77.9 (2)	F2A—C2A—F1A	106.2 (8)
O2F^{ii}—Ba2—O2B	152.0 (2)	F2A—C2A—C1A	112.8 (8)
O2G—Ba2—O1C	135.2 (2)	F1A—C2A—C1A	112.4 (8)
O1F—Ba2—O1C	103.04 (19)	F2A—C2A—Br1A	107.2 (7)
O2F^{ii}—Ba2—O1C	88.6 (2)	F1A—C2A—Br1A	108.6 (6)
O2B—Ba2—O1C	72.0 (2)	C1A—C2A—Br1A	109.4 (6)
O2G—Ba2—O2E^{ii}	71.6 (2)	C1A—O2A—Ba5^{iii}	153.4 (6)
O1F—Ba2—O2E^{ii}	151.19 (19)	C1B—O1B—Ba3	91.8 (6)

O2F^{ii}—Ba2—O2E^{ii}	80.0 (2)	O1B—C1B—O2B	128.5 (9)
O2B—Ba2—O2E^{ii}	73.6 (2)	O1B—C1B—C2B	116.8 (8)
O1C—Ba2—O2E^{ii}	64.3 (2)	O2B—C1B—C2B	114.7 (8)
O2G—Ba2—O4W	95.3 (2)	O1B—C1B—Ba3	65.5 (5)
O1F—Ba2—O4W	67.5 (2)	O2B—C1B—Ba3	63.0 (5)
O2F^{ii}—Ba2—O4W	60.8 (2)	C2B—C1B—Ba3	177.7 (7)
O2B—Ba2—O4W	145.4 (2)	C1B—O2B—Ba2	169.0 (6)
O1C—Ba2—O4W	113.6 (2)	C1B—O2B—Ba3	94.1 (5)
O2E^{ii}—Ba2—O4W	140.7 (2)	Ba2—O2B—Ba3	96.9 (2)
O2G—Ba2—F2F	67.2 (2)	F2B—C2B—F1B	107.6 (10)
O1F—Ba2—F2F	53.2 (2)	F2B—C2B—C1B	113.4 (8)
O2F^{ii}—Ba2—F2F	122.1 (2)	F1B—C2B—C1B	110.8 (9)
O2B—Ba2—F2F	81.5 (2)	F2B—C2B—Br1B	107.5 (8)
O1C—Ba2—F2F	148.2 (2)	F1B—C2B—Br1B	106.7 (7)
O2E^{ii}—Ba2—F2F	124.7 (2)	C1B—C2B—Br1B	110.5 (8)
O4W—Ba2—F2F	79.2 (2)	C1C—O1C—Ba3	135.3 (6)
O2G—Ba2—O2C	167.5 (2)	C1C—O1C—Ba2	104.6 (6)
O1F—Ba2—O2C	66.84 (19)	Ba3—O1C—Ba2	100.4 (2)
O2F^{ii}—Ba2—O2C	91.3 (2)	O2C—C1C—O1C	125.8 (9)
O2B—Ba2—O2C	88.4 (2)	O2C—C1C—C2C	118.1 (9)
O1C—Ba2—O2C	43.91 (18)	O1C—C1C—C2C	116.0 (9)
O2E^{ii}—Ba2—O2C	107.9 (2)	O2C—C1C—Ba2	72.1 (6)
O4W—Ba2—O2C	77.1 (2)	O1C—C1C—Ba2	53.7 (5)
F2F—Ba2—O2C	120.05 (18)	C2C—C1C—Ba2	169.6 (7)
O2G—Ba2—F3G	48.6 (6)	C1C—O2C—Ba1	152.5 (6)
O1F—Ba2—F3G	81.3 (5)	C1C—O2C—Ba2	85.6 (6)
O2F^{ii}—Ba2—F3G	123.8 (7)	Ba1—O2C—Ba2	104.0 (2)
O2B—Ba2—F3G	66.3 (9)	F2C—C2C—F1C	105.8 (8)
O1C—Ba2—F3G	136.2 (10)	F2C—C2C—C1C	112.3 (9)
O2E^{ii}—Ba2—F3G	90.9 (8)	F1C—C2C—C1C	112.3 (8)
O4W—Ba2—F3G	108.3 (10)	F2C—C2C—Br1C	108.1 (7)
O2C—Ba2—F3G	143.1 (5)	F1C—C2C—Br1C	107.3 (7)
O2G—Ba2—C1C	154.9 (2)	C1C—C2C—Br1C	110.8 (7)
O1F—Ba2—C1C	85.2 (2)	C2D—O1D—Ba1	153.1 (6)
O2F^{ii}—Ba2—C1C	89.5 (2)	C2D—O1D—Ba5^{vii}	93.6 (6)
O2B—Ba2—C1C	79.7 (2)	Ba1—O1D—Ba5^{vii}	106.6 (2)
O1C—Ba2—C1C	21.7 (2)	F2D—C1D—F1D	108.0 (8)

O2E^{ii}—Ba2—C1C	85.8 (2)	F2D—C1D—C2D	111.2 (7)
O4W—Ba2—C1C	95.5 (2)	F1D—C1D—C2D	111.2 (8)
F2F—Ba2—C1C	137.2 (2)	F2D—C1D—Br2D	108.0 (6)
O2C—Ba2—C1C	22.2 (2)	F1D—C1D—Br2D	108.4 (6)
F3G—Ba2—C1C	145.4 (9)	C2D—C1D—Br2D	109.8 (6)
O2G—Ba2—Ba3	107.63 (19)	O2D—C2D—O1D	126.6 (9)
O1F—Ba2—Ba3	110.75 (14)	O2D—C2D—C1D	116.1 (8)
O2F^{ii}—Ba2—Ba3	110.12 (15)	O1D—C2D—C1D	117.3 (8)
O2B—Ba2—Ba3	42.66 (14)	O2D—C2D—Ba5^{vii}	64.0 (5)
O1C—Ba2—Ba3	39.25 (14)	O1D—C2D—Ba5^{vii}	63.5 (5)
O2E^{ii}—Ba2—Ba3	42.66 (14)	C1D—C2D—Ba5^{vii}	169.0 (6)
O4W—Ba2—Ba3	152.84 (17)	C2D—O2D—Ba4^{vii}	150.5 (6)
F2F—Ba2—Ba3	122.74 (15)	C2D—O2D—Ba5^{vii}	93.4 (5)
O2C—Ba2—Ba3	77.63 (13)	Ba4^{vii}—O2D—Ba5^{vii}	108.7 (2)
F3G—Ba2—Ba3	97.9 (10)	C1E—O1E—Ba1	144.5 (6)
C1C—Ba2—Ba3	57.73 (17)	C1E—O2E—Ba2^{i}	128.4 (6)
O1C—Ba3—O1J	114.6 (2)	C1E—O2E—Ba3^{i}	133.1 (6)
O1C—Ba3—O1A	177.9 (2)	Ba2^{i}—O2E—Ba3^{i}	95.70 (19)
O1J—Ba3—O1A	65.78 (19)	O1E—C1E—O2E	130.8 (9)
O1C—Ba3—O2H	68.94 (19)	O1E—C1E—C2E	113.7 (8)
O1J—Ba3—O2H	103.5 (2)	O2E—C1E—C2E	115.5 (8)
O1A—Ba3—O2H	108.94 (19)	O1E—C1E—C3E	113.3 (14)
O1C—Ba3—O2E^{ii}	64.3 (2)	O2E—C1E—C3E	111.9 (12)
O1J—Ba3—O2E^{ii}	118.30 (19)	F1E—C2E—F2E	107.2 (9)
O1A—Ba3—O2E^{ii}	117.55 (19)	F1E—C2E—C1E	110.7 (9)
O2H—Ba3—O2E^{ii}	126.54 (19)	F2E—C2E—C1E	111.4 (8)
O1C—Ba3—O2B	71.1 (2)	F1E—C2E—Br1E	109.0 (8)
O1J—Ba3—O2B	170.35 (18)	F2E—C2E—Br1E	107.8 (7)
O1A—Ba3—O2B	108.30 (19)	C1E—C2E—Br1E	110.5 (8)
O2H—Ba3—O2B	70.6 (2)	C2E—F2E—Ba3^{i}	124.0 (5)
O2E^{ii}—Ba3—O2B	70.96 (19)	F3E—C3E—F4E	108 (2)
O1C—Ba3—O1H	109.5 (2)	F3E—C3E—C1E	110 (2)
O1J—Ba3—O1H	67.37 (19)	F4E—C3E—C1E	110.2 (19)
O1A—Ba3—O1H	68.6 (2)	F3E—C3E—Br2E	108.9 (18)
O2H—Ba3—O1H	46.08 (19)	F4E—C3E—Br2E	106.2 (17)
O2E^{ii}—Ba3—O1H	172.62 (19)	C1E—C3E—Br2E	113.5 (13)
O2B—Ba3—O1H	103.65 (19)	C1F—O1F—Ba2	137.1 (6)

O1C—Ba3—O1B	110.8 (2)	C1F—O1F—Ba1	105.6 (6)
O1J—Ba3—O1B	125.37 (19)	Ba2—O1F—Ba1	115.3 (2)
O1A—Ba3—O1B	67.82 (18)	C1F—O2F—Ba2^{i}	154.8 (6)
O2H—Ba3—O1B	66.6 (2)	C1F—O2F—Ba1	81.6 (6)
O2E^{ii}—Ba3—O1B	107.7 (2)	Ba2^{i}—O2F—Ba1	101.8 (3)
O2B—Ba3—O1B	45.62 (18)	O2F—C1F—O1F	128.2 (10)
O1H—Ba3—O1B	70.1 (2)	O2F—C1F—C3F	103.8 (14)
O1C—Ba3—F1A	126.80 (19)	O1F—C1F—C3F	128.0 (14)
O1J—Ba3—F1A	105.48 (19)	O2F—C1F—C2F	119.0 (9)
O1A—Ba3—F1A	54.48 (17)	O1F—C1F—C2F	112.7 (8)
O2H—Ba3—F1A	133.46 (19)	O2F—C1F—Ba1	76.9 (6)
O2E^{ii}—Ba3—F1A	66.49 (18)	O1F—C1F—Ba1	53.3 (5)
O2B—Ba3—F1A	75.1 (2)	C3F—C1F—Ba1	165.5 (10)
O1H—Ba3—F1A	117.64 (19)	C2F—C1F—Ba1	156.8 (7)
O1B—Ba3—F1A	66.93 (18)	F2F—C2F—F1F	106.1 (10)
O1C—Ba3—F1J	69.80 (19)	F2F—C2F—C1F	111.4 (9)
O1J—Ba3—F1J	52.68 (17)	F1F—C2F—C1F	110.1 (10)
O1A—Ba3—F1J	111.47 (17)	F2F—C2F—Br1F	108.3 (8)
O2H—Ba3—F1J	111.6 (2)	F1F—C2F—Br1F	109.8 (8)
O2E^{ii}—Ba3—F1J	74.88 (19)	C1F—C2F—Br1F	110.9 (8)
O2B—Ba3—F1J	136.18 (17)	C2F—F2F—Ba2	120.2 (7)
O1H—Ba3—F1J	107.3 (2)	F4F—C3F—F3F	108 (2)
O1B—Ba3—F1J	177.4 (2)	F4F—C3F—C1F	110.9 (19)
F1A—Ba3—F1J	114.88 (19)	F3F—C3F—C1F	110.3 (19)
O1C—Ba3—F2E^{ii}	101.38 (18)	F4F—C3F—Br2F	108.9 (18)
O1J—Ba3—F2E^{ii}	70.08 (18)	F3F—C3F—Br2F	112.0 (18)
O1A—Ba3—F2E^{ii}	80.72 (18)	C1F—C3F—Br2F	106.5 (14)
O2H—Ba3—F2E^{ii}	165.6 (2)	C1G—O1G—Ba5^{viii}	158.9 (7)
O2E^{ii}—Ba3—F2E^{ii}	52.30 (17)	C1G—O1G—Ba1^{ii}	89.8 (6)
O2B—Ba3—F2E^{ii}	117.42 (18)	Ba5^{viii}—O1G—Ba1^{ii}	105.7 (2)
O1H—Ba3—F2E^{ii}	134.77 (17)	C1G—O2G—Ba2	147.4 (7)
O1B—Ba3—F2E^{ii}	127.7 (2)	C1G—O2G—Ba1^{ii}	94.7 (6)
F1A—Ba3—F2E^{ii}	60.84 (17)	Ba2—O2G—Ba1^{ii}	116.5 (3)
F1J—Ba3—F2E^{ii}	54.0 (2)	O1G—C1G—O2G	129.1 (10)
O1C—Ba3—F4E^{ii}	109.0 (5)	O1G—C1G—C3G	120 (2)
O1J—Ba3—F4E^{ii}	81.1 (8)	O2G—C1G—C3G	109 (2)
O1A—Ba3—F4E^{ii}	73.1 (5)	O1G—C1G—C2G	115.7 (9)

O2H—Ba3—F4E^{ii}	175.4 (8)	O2G—C1G—C2G	115.1 (9)
O2E^{ii}—Ba3—F4E^{ii}	49.7 (5)	O1G—C1G—Ba1^{ii}	67.8 (6)
O2B—Ba3—F4E^{ii}	104.9 (9)	O2G—C1G—Ba1^{ii}	62.7 (5)
O1H—Ba3—F4E^{ii}	137.7 (5)	C2G—C1G—Ba1^{ii}	166.4 (7)
O1B—Ba3—F4E^{ii}	111.1 (9)	F2G—C2G—F1G	106.7 (8)
F1A—Ba3—F4E^{ii}	44.2 (9)	F2G—C2G—C1G	110.9 (9)
F1J—Ba3—F4E^{ii}	70.7 (9)	F1G—C2G—C1G	111.6 (9)
F2E^{ii}—Ba3—F4E^{ii}	16.8 (9)	F2G—C2G—Br1G	108.8 (7)
O1I—Ba4—O3I^{iii}	127.8 (2)	F1G—C2G—Br1G	107.9 (7)
O1I—Ba4—O1H	148.5 (2)	C1G—C2G—Br1G	110.8 (7)
O3I^{iii}—Ba4—O1H	79.2 (2)	F4G—C3G—F3G	109 (2)
O1I—Ba4—O2D^{iv}	77.1 (2)	F4G—C3G—C1G	113 (2)
O3I^{iii}—Ba4—O2D^{iv}	121.8 (2)	F3G—C3G—C1G	114 (2)
O1H—Ba4—O2D^{iv}	103.7 (2)	F4G—C3G—Br2G	110.4 (19)
O1I—Ba4—O1J	79.9 (2)	F3G—C3G—Br2G	108.8 (19)
O3I^{iii}—Ba4—O1J	145.2 (2)	C1G—C3G—Br2G	101.8 (13)
O1H—Ba4—O1J	69.3 (2)	C3G—F3G—Ba2	114 (3)
O2D^{iv}—Ba4—O1J	81.1 (2)	C1H—O2H—Ba3	95.1 (6)
O1I—Ba4—O1A	90.5 (2)	C1H—O1H—Ba4	166.9 (7)
O3I^{iii}—Ba4—O1A	92.1 (2)	C1H—O1H—Ba3	92.3 (6)
O1H—Ba4—O1A	70.5 (2)	Ba4—O1H—Ba3	100.6 (2)
O2D^{iv}—Ba4—O1A	144.64 (19)	O2H—C1H—O1H	126.1 (9)
O1J—Ba4—O1A	64.09 (19)	O2H—C1H—C2H	118.2 (9)
O1I—Ba4—O6W	65.8 (2)	O1H—C1H—C2H	115.6 (9)
O3I^{iii}—Ba4—O6W	75.1 (2)	O2H—C1H—C3H	113.2 (14)
O1H—Ba4—O6W	145.0 (2)	O1H—C1H—C3H	117.8 (14)
O2D^{iv}—Ba4—O6W	71.3 (2)	O2H—C1H—Ba3	62.0 (5)
O1J—Ba4—O6W	139.68 (19)	O1H—C1H—Ba3	64.4 (5)
O1A—Ba4—O6W	133.2 (2)	C2H—C1H—Ba3	177.4 (7)
O1I—Ba4—O5W	70.4 (2)	C3H—C1H—Ba3	156.2 (10)
O3I^{iii}—Ba4—O5W	59.9 (2)	F2H—C2H—F1H	106.7 (11)
O1H—Ba4—O5W	125.4 (2)	F2H—C2H—C1H	113.7 (9)
O2D^{iv}—Ba4—O5W	127.7 (2)	F1H—C2H—C1H	113.7 (9)
O1J—Ba4—O5W	129.5 (2)	F2H—C2H—Br1H	107.6 (8)
O1A—Ba4—O5W	76.08 (19)	F1H—C2H—Br1H	108.9 (8)
O6W—Ba4—O5W	58.4 (2)	C1H—C2H—Br1H	106.1 (8)
O1I—Ba4—F1I^{iii}	127.09 (18)	F3H—C3H—F4H	105 (2)

O3I^{iii}—Ba4—F1I^{iii}	50.60 (19)	F3H—C3H—C1H	118 (2)
O1H—Ba4—F1I^{iii}	81.27 (19)	F4H—C3H—C1H	116 (2)
O2D^{iv}—Ba4—F1I^{iii}	72.03 (17)	F3H—C3H—Br2H	108.9 (18)
O1J—Ba4—F1I^{iii}	133.75 (18)	F4H—C3H—Br2H	107.1 (18)
O1A—Ba4—F1I^{iii}	137.32 (16)	C1H—C3H—Br2H	101.0 (11)
O6W—Ba4—F1I^{iii}	64.05 (17)	O1I—C1I—O3I	127.2 (10)
O5W—Ba4—F1I^{iii}	96.51 (17)	O1I—C1I—C2I	117.7 (8)
O1I—Ba4—Ba3	108.57 (15)	O3I—C1I—C2I	115.0 (8)
O3I^{iii}—Ba4—Ba3	106.28 (16)	O1I—C1I—Ba5	71.6 (6)
O1H—Ba4—Ba3	41.43 (16)	O3I—C1I—Ba5	59.3 (5)
O2D^{iv}—Ba4—Ba3	113.00 (15)	C2I—C1I—Ba5	156.6 (6)
O1J—Ba4—Ba3	39.24 (13)	C2I—F1I—Ba4^{v}	115.4 (5)
O1A—Ba4—Ba3	39.99 (13)	C1I—O1I—Ba4	157.7 (7)
O6W—Ba4—Ba3	172.51 (15)	C1I—O1I—Ba5	86.3 (6)
O5W—Ba4—Ba3	115.62 (14)	Ba4—O1I—Ba5	105.0 (2)
F1I^{iii}—Ba4—Ba3	122.67 (11)	F1I—C2I—F2I	106.7 (8)
O1I—Ba4—Ba5	41.13 (17)	F1I—C2I—C1I	111.8 (8)
O3I^{iii}—Ba4—Ba5	143.54 (16)	F2I—C2I—C1I	111.9 (8)
O1H—Ba4—Ba5	127.46 (17)	F1I—C2I—Br1I	108.6 (6)
O2D^{iv}—Ba4—Ba5	37.05 (14)	F2I—C2I—Br1I	108.4 (6)
O1J—Ba4—Ba5	70.72 (13)	C1I—C2I—Br1I	109.3 (6)
O1A—Ba4—Ba5	118.52 (13)	C1I—O3I—Ba4^{v}	143.4 (7)
O6W—Ba4—Ba5	69.52 (13)	C1I—O3I—Ba5	98.6 (6)
O5W—Ba4—Ba5	106.22 (12)	Ba4^{v}—O3I—Ba5	117.7 (2)
F1I^{iii}—Ba4—Ba5	103.99 (10)	C1J—O1J—Ba3	136.5 (6)
Ba3—Ba4—Ba5	109.946 (15)	C1J—O1J—Ba4	123.0 (6)
O1I—Ba4—Ba5^{iii}	105.84 (16)	Ba3—O1J—Ba4	100.4 (2)
O3I^{iii}—Ba4—Ba5^{iii}	32.27 (16)	C1J—O2J—Ba5	158.6 (7)
O1H—Ba4—Ba5^{iii}	90.01 (17)	O2J—C1J—O1J	129.2 (9)
O2D^{iv}—Ba4—Ba5^{iii}	148.11 (15)	O2J—C1J—C2J	115.2 (9)
O1J—Ba4—Ba5^{iii}	130.82 (14)	O1J—C1J—C2J	115.6 (9)
O1A—Ba4—Ba5^{iii}	67.02 (13)	F2J—C2J—F1J	105.9 (9)
O6W—Ba4—Ba5^{iii}	80.87 (14)	F2J—C2J—C1J	111.0 (9)
O5W—Ba4—Ba5^{iii}	36.52 (12)	F1J—C2J—C1J	111.2 (8)
F1I^{iii}—Ba4—Ba5^{iii}	82.05 (10)	F2J—C2J—Br1J	108.1 (7)
Ba3—Ba4—Ba5^{iii}	96.414 (14)	F1J—C2J—Br1J	107.4 (7)
Ba5—Ba4—Ba5^{iii}	142.428 (13)	C1J—C2J—Br1J	113.0 (7)

O2J—Ba5—O2A^{v}	150.7 (2)	C2J—F1J—Ba3	123.5 (5)
O2J—Ba5—O1G^{vi}	101.0 (2)	Ba1—O1W—Ba5^{vii}	95.9 (2)
O2A^{v}—Ba5—O1G^{vi}	71.1 (2)	Ba5^{iii}—O5W—Ba4	105.4 (2)
O2A—C1A—O1A—Ba3	−129.2 (9)	O1F—C1F—C2F—F1F	137.9 (10)
C2A—C1A—O1A—Ba3	50.2 (10)	Ba1—C1F—C2F—F1F	−174.2 (12)
O2A—C1A—O1A—Ba4	5.8 (14)	O2F—C1F—C2F—Br1F	77.4 (11)
C2A—C1A—O1A—Ba4	−174.8 (5)	O1F—C1F—C2F—Br1F	−100.3 (9)
Ba3—F1A—C2A—F2A	108.3 (7)	Ba1—C1F—C2F—Br1F	−52 (2)
Ba3—F1A—C2A—C1A	−15.5 (9)	F1F—C2F—F2F—Ba2	−146.7 (7)
Ba3—F1A—C2A—Br1A	−136.7 (4)	C1F—C2F—F2F—Ba2	−26.8 (12)
O2A—C1A—C2A—F2A	39.5 (12)	Br1F—C2F—F2F—Ba2	95.4 (7)
O1A—C1A—C2A—F2A	−140.0 (8)	O2F—C1F—C3F—F4F	−132 (2)
O2A—C1A—C2A—F1A	159.5 (8)	O1F—C1F—C3F—F4F	47 (3)
O1A—C1A—C2A—F1A	−20.0 (12)	Ba1—C1F—C3F—F4F	137 (5)
O2A—C1A—C2A—Br1A	−79.7 (9)	O2F—C1F—C3F—F3F	−12 (2)
O1A—C1A—C2A—Br1A	100.8 (8)	O1F—C1F—C3F—F3F	167 (2)
O1A—C1A—O2A—Ba5^{iii}	10 (2)	Ba1—C1F—C3F—F3F	−103 (5)
C2A—C1A—O2A—Ba5^{iii}	−169.0 (10)	O2F—C1F—C3F—Br2F	109.4 (17)
Ba3—O1B—C1B—O2B	2.0 (12)	O1F—C1F—C3F—Br2F	−71 (2)
Ba3—O1B—C1B—C2B	179.9 (8)	Ba1—C1F—C3F—Br2F	18 (6)
O1B—C1B—O2B—Ba2	170 (3)	Ba5^{viii}—O1G—C1G—O2G	151.3 (13)
C2B—C1B—O2B—Ba2	−8 (4)	Ba1^{ii}—O1G—C1G—O2G	13.5 (12)
Ba3—C1B—O2B—Ba2	172 (4)	Ba5^{viii}—O1G—C1G—C3G	−46 (3)
O1B—C1B—O2B—Ba3	−2.0 (12)	Ba1^{ii}—O1G—C1G—C3G	176.0 (13)
C2B—C1B—O2B—Ba3	−180.0 (8)	Ba5^{viii}—O1G—C1G—C2G	−28 (2)
O1B—C1B—C2B—F2B	−154.2 (10)	Ba1^{ii}—O1G—C1G—C2G	−165.6 (8)
O2B—C1B—C2B—F2B	24.0 (14)	Ba5^{viii}—O1G—C1G—Ba1^{ii}	137.8 (19)
O1B—C1B—C2B—F1B	−33.0 (13)	Ba2—O2G—C1G—O1G	−178.0 (8)
O2B—C1B—C2B—F1B	145.2 (9)	Ba1^{ii}—O2G—C1G—O1G	−14.1 (13)
O1B—C1B—C2B—Br1B	85.0 (10)	Ba2—O2G—C1G—C3G	18 (2)
O2B—C1B—C2B—Br1B	−96.8 (9)	Ba1^{ii}—O2G—C1G—C3G	−178.0 (12)
Ba3—O1C—C1C—O2C	−119.7 (10)	Ba2—O2G—C1G—C2G	1.2 (19)
Ba2—O1C—C1C—O2C	2.1 (11)	Ba1^{ii}—O2G—C1G—C2G	165.1 (7)
Ba3—O1C—C1C—C2C	60.3 (11)	Ba2—O2G—C1G—Ba1^{ii}	−163.8 (14)
Ba2—O1C—C1C—C2C	−177.8 (7)	O1G—C1G—C2G—F2G	−63.7 (12)
Ba3—O1C—C1C—Ba2	−121.9 (8)	O2G—C1G—C2G—F2G	117.0 (11)

O1C—C1C—O2C—Ba1	110.4 (15)	Ba1^{ii}—C1G—C2G—F2G	−166 (2)
C2C—C1C—O2C—Ba1	−69.6 (18)	O1G—C1G—C2G—F1G	177.5 (9)
Ba2—C1C—O2C—Ba1	112.2 (14)	O2G—C1G—C2G—F1G	−1.8 (13)
O1C—C1C—O2C—Ba2	−1.8 (9)	Ba1^{ii}—C1G—C2G—F1G	76 (3)
C2C—C1C—O2C—Ba2	178.2 (8)	O1G—C1G—C2G—Br1G	57.2 (11)
O2C—C1C—C2C—F2C	167.1 (8)	O2G—C1G—C2G—Br1G	−122.1 (9)
O1C—C1C—C2C—F2C	−12.9 (12)	Ba1^{ii}—C1G—C2G—Br1G	−45 (3)
Ba2—C1C—C2C—F2C	−23 (4)	O1G—C1G—C3G—F4G	−29 (3)
O2C—C1C—C2C—F1C	48.1 (12)	O2G—C1G—C3G—F4G	137 (3)
O1C—C1C—C2C—F1C	−131.9 (9)	O1G—C1G—C3G—F3G	−154 (3)
Ba2—C1C—C2C—F1C	−142 (3)	O2G—C1G—C3G—F3G	12 (3)
O2C—C1C—C2C—Br1C	−71.9 (10)	O1G—C1G—C3G—Br2G	89 (2)
O1C—C1C—C2C—Br1C	108.1 (8)	O2G—C1G—C3G—Br2G	−105 (2)
Ba2—C1C—C2C—Br1C	98 (4)	F4G—C3G—F3G—Ba2	−151 (3)
Ba1—O1D—C2D—O2D	−128.1 (13)	C1G—C3G—F3G—Ba2	−24 (3)
Ba5^{vii}—O1D—C2D—O2D	11.2 (11)	Br2G—C3G—F3G—Ba2	89 (2)
Ba1—O1D—C2D—C1D	53.0 (18)	Ba3—O2H—C1H—O1H	6.2 (11)
Ba5^{vii}—O1D—C2D—C1D	−167.7 (7)	Ba3—O2H—C1H—C2H	−177.0 (8)
Ba1—O1D—C2D—Ba5^{vii}	−139.3 (15)	Ba3—O2H—C1H—C3H	−154.0 (10)
F2D—C1D—C2D—O2D	47.4 (12)	Ba4—O1H—C1H—O2H	165 (2)
F1D—C1D—C2D—O2D	167.8 (8)	Ba3—O1H—C1H—O2H	−6.1 (11)
Br2D—C1D—C2D—O2D	−72.1 (9)	Ba4—O1H—C1H—C2H	−12 (4)
F2D—C1D—C2D—O1D	−133.6 (9)	Ba3—O1H—C1H—C2H	177.1 (8)
F1D—C1D—C2D—O1D	−13.1 (12)	Ba4—O1H—C1H—C3H	−36 (4)
Br2D—C1D—C2D—O1D	106.9 (9)	Ba3—O1H—C1H—C3H	153.4 (11)
F2D—C1D—C2D—Ba5^{vii}	135 (3)	Ba4—O1H—C1H—Ba3	171 (3)
F1D—C1D—C2D—Ba5^{vii}	−105 (3)	O2H—C1H—C2H—F2H	−153.3 (10)
Br2D—C1D—C2D—Ba5^{vii}	15 (4)	O1H—C1H—C2H—F2H	23.8 (14)
O1D—C2D—O2D—Ba4^{vii}	−150.3 (9)	O2H—C1H—C2H—F1H	−30.9 (15)
C1D—C2D—O2D—Ba4^{vii}	28.6 (17)	O1H—C1H—C2H—F1H	146.2 (10)
Ba5^{vii}—C2D—O2D—Ba4^{vii}	−139.1 (13)	O2H—C1H—C2H—Br1H	88.7 (10)
O1D—C2D—O2D—Ba5^{vii}	−11.2 (11)	O1H—C1H—C2H—Br1H	−94.2 (9)
C1D—C2D—O2D—Ba5^{vii}	167.7 (7)	O2H—C1H—C3H—F3H	35 (2)
Ba1—O1E—C1E—O2E	−43.2 (19)	O1H—C1H—C3H—F3H	−127 (2)
Ba1—O1E—C1E—C2E	136.0 (9)	Ba3—C1H—C3H—F3H	−38 (4)
Ba1—O1E—C1E—C3E	112.2 (14)	O2H—C1H—C3H—F4H	161 (2)
Ba2^{i}—O2E—C1E—O1E	−1.6 (17)	O1H—C1H—C3H—F4H	−1 (2)

Ba3^{i}—O2E—C1E—O1E	−157.8 (8)	Ba3—C1H—C3H—F4H	88 (3)
Ba2^{i}—O2E—C1E—C2E	179.1 (6)	O2H—C1H—C3H—Br2H	−83.8 (15)
Ba3^{i}—O2E—C1E—C2E	22.9 (14)	O1H—C1H—C3H—Br2H	114.1 (14)
Ba2^{i}—O2E—C1E—C3E	−157.4 (13)	Ba3—C1H—C3H—Br2H	−157 (2)
Ba3^{i}—O2E—C1E—C3E	46.4 (16)	O3I—C1I—O1I—Ba4	143.5 (13)
O1E—C1E—C2E—F1E	40.6 (13)	C2I—C1I—O1I—Ba4	−35 (2)
O2E—C1E—C2E—F1E	−140.0 (10)	Ba5—C1I—O1I—Ba4	121.8 (17)
O1E—C1E—C2E—F2E	159.9 (9)	O3I—C1I—O1I—Ba5	21.7 (10)
O2E—C1E—C2E—F2E	−20.8 (13)	C2I—C1I—O1I—Ba5	−156.6 (8)
O1E—C1E—C2E—Br1E	−80.3 (10)	Ba4^{v}—F1I—C2I—F2I	−141.3 (6)
O2E—C1E—C2E—Br1E	99.1 (9)	Ba4^{v}—F1I—C2I—C1I	−18.6 (9)
F1E—C2E—F2E—Ba3^{i}	133.9 (7)	Ba4^{v}—F1I—C2I—Br1I	102.1 (5)
C1E—C2E—F2E—Ba3^{i}	12.7 (12)	O1I—C1I—C2I—F1I	−159.5 (8)
Br1E—C2E—F2E—Ba3^{i}	−108.8 (6)	O3I—C1I—C2I—F1I	22.0 (12)
O1E—C1E—C3E—F3E	−65 (2)	Ba5—C1I—C2I—F1I	92.0 (16)
O2E—C1E—C3E—F3E	95 (2)	O1I—C1I—C2I—F2I	−39.9 (12)
O1E—C1E—C3E—F4E	176 (2)	O3I—C1I—C2I—F2I	141.6 (8)
O2E—C1E—C3E—F4E	−24 (2)	Ba5—C1I—C2I—F2I	−148.3 (12)
O1E—C1E—C3E—Br2E	57 (2)	O1I—C1I—C2I—Br1I	80.3 (9)
O2E—C1E—C3E—Br2E	−142.6 (15)	O3I—C1I—C2I—Br1I	−98.3 (8)
F3E—C3E—F4E—Ba3^{i}	−120 (3)	Ba5—C1I—C2I—Br1I	−28.2 (17)
C1E—C3E—F4E—Ba3^{i}	0 (3)	O1I—C1I—O3I—Ba4^{v}	164.4 (7)
Br2E—C3E—F4E—Ba3^{i}	124 (2)	C2I—C1I—O3I—Ba4^{v}	−17.3 (15)
Ba2^{i}—O2F—C1F—O1F	115.1 (16)	Ba5—C1I—O3I—Ba4^{v}	−171.5 (11)
Ba1—O2F—C1F—O1F	15.4 (10)	O1I—C1I—O3I—Ba5	−24.1 (11)
Ba2^{i}—O2F—C1F—C3F	−65 (2)	C2I—C1I—O3I—Ba5	154.2 (7)
Ba1—O2F—C1F—C3F	−165.1 (11)	Ba5—O2J—C1J—O1J	−20 (3)
Ba2^{i}—O2F—C1F—C2F	−62 (2)	Ba5—O2J—C1J—C2J	157.3 (16)
Ba1—O2F—C1F—C2F	−161.9 (9)	Ba3—O1J—C1J—O2J	−172.9 (8)
Ba2^{i}—O2F—C1F—Ba1	99.8 (16)	Ba4—O1J—C1J—O2J	10.0 (16)
Ba2—O1F—C1F—O2F	178.8 (7)	Ba3—O1J—C1J—C2J	10.1 (15)
Ba1—O1F—C1F—O2F	−18.8 (12)	Ba4—O1J—C1J—C2J	−167.0 (7)
Ba2—O1F—C1F—C3F	−0.6 (18)	O2J—C1J—C2J—F2J	−65.0 (13)
Ba1—O1F—C1F—C3F	161.8 (13)	O1J—C1J—C2J—F2J	112.4 (11)
Ba2—O1F—C1F—C2F	−3.8 (13)	O2J—C1J—C2J—F1J	177.4 (10)
Ba1—O1F—C1F—C2F	158.6 (7)	O1J—C1J—C2J—F1J	−5.2 (14)
Ba2—O1F—C1F—Ba1	−162.4 (9)	O2J—C1J—C2J—Br1J	56.5 (12)

O2F—C1F—C2F—F2F	−162.0 (9)	O1J—C1J—C2J—Br1J	−126.1 (9)
O1F—C1F—C2F—F2F	20.4 (13)	F2J—C2J—F1J—Ba3	−120.5 (7)
Ba1—C1F—C2F—F2F	68.3 (19)	C1J—C2J—F1J—Ba3	0.2 (12)
O2F—C1F—C2F—F1F	−44.5 (13)	Br1J—C2J—F1J—Ba3	124.3 (5)

Symmetry codes: (i) *x*+1/2, −*y*+1/2, −*z*+1; (ii) *x*−1/2, −*y*+1/2, −*z*+1; (iii) *x*+1/2, −*y*+1/2, −*z*+2; (iv) −*x*+1/2, −*y*, *z*+1/2; (v) *x*−1/2, −*y*+1/2, −*z*+2; (vi) −*x*, *y*−1/2, −*z*+3/2; (vii) −*x*+1/2, −*y*, *z*−1/2; (viii) −*x*, *y*+1/2, −*z*+3/2.

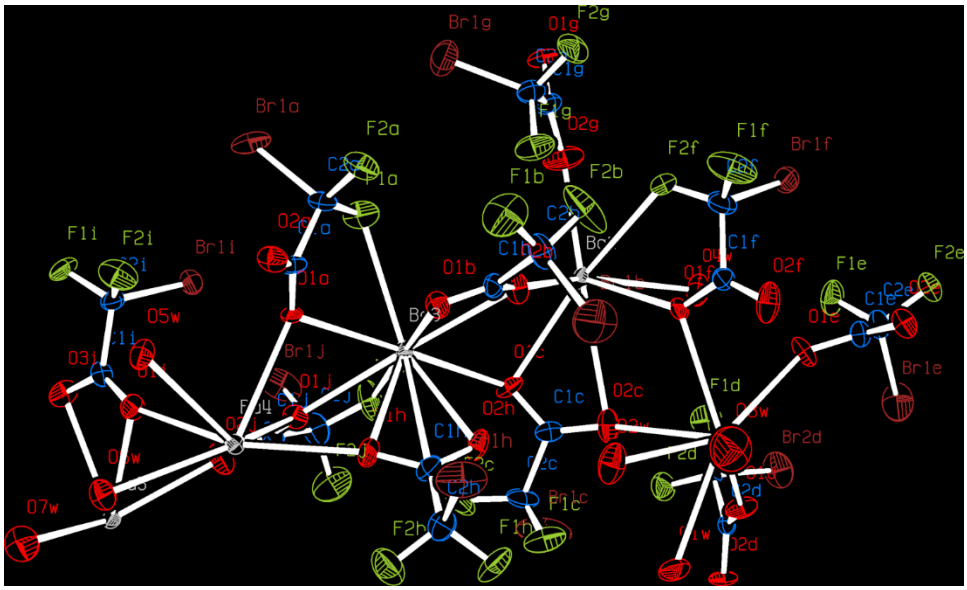

Figure S1. Thermal ellipsoids (70% probability). Atom splitting is not shown for clarity.

2. Powder X-ray Diffraction of BaFBr

Table S5. Results from Rietveld Analyses of PXRD Patterns of BaFBr

	Solid-State Thermolysis	Solution-Phase Thermolysis
a (Å)	4.5118 (3)	4.5012 (6)
c (Å)	7.4456 (5)	7.4796 (14)
V (Å^3)	151.57 (3)	151.54 (6)
zBa	0.1923 (4)	0.1947 (4)
zBr	0.6489 (5)	0.6473 (6)
$100 \times U^{iso}$	0.125	1.30 (16)
R_{wp} (%)	10.0	11.3

3. Powder X-ray Diffraction of Yb:Er:BaFBr Nanocrystals

Table S6. Results from Rietveld Analysis of the PXRD Pattern of Yb:Er:BaFBr Nanocrystals (3.00 mol. %)

a (Å)	4.4851 (9)
c (Å)	7.559 (3)
V (Å^3)	152.06 (10)
zM[a]	0.1971 (4)
zBr	0.6446 (7)
$100 \times U^{iso}$	0.11 (13)
R_{wp} (%)	9.2

[a]Occupancy of the metal site (M): Yb:Er:Ba = 0.01983:0.00157:0.9786.

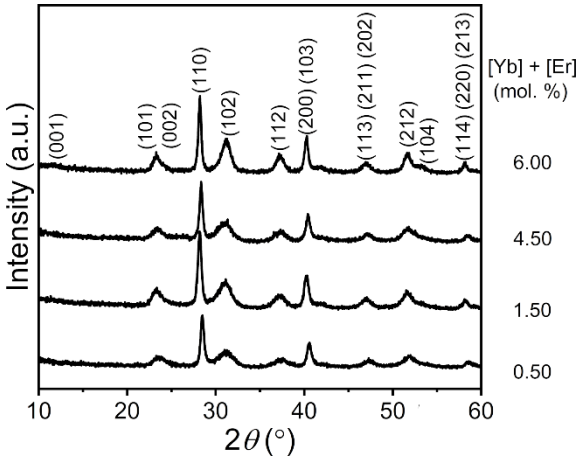

Figure S2. PXRD patterns of Yb:Er:BaFBr nanocrystals. Nominal total rare-earth concentrations are indicated.

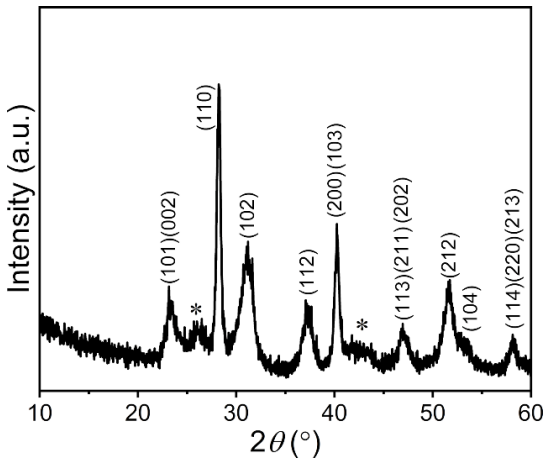

Figure S3. PXRD pattern of Yb:Er:BaFBr nanocrystals with a nominal rare-earth concentration of 7.5 mol %. Diffraction maxima corresponding to secondary phases are depicted with ⁎.

4. Transmission Electron Microscopy Imaging of Yb:Er:BaFBr Nanocrystals

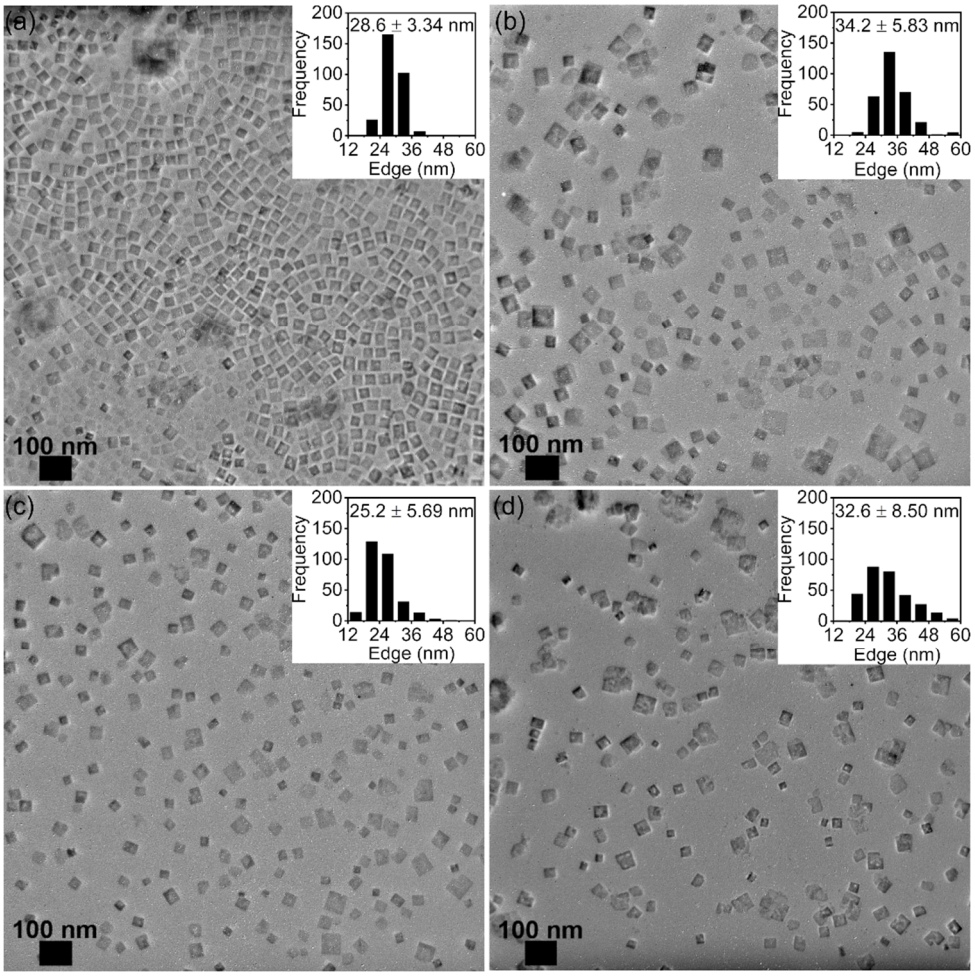

Figure S4. TEM images and size distribution histograms of Yb:Er:BaFBr nanocrystals featuring nominal total rare-earth concentrations of 0.50 (a), 1.5 (b), 4.5 (c), and 6.0 mol. % (d).

5. Elemental Analysis of Yb:Er:BaFBr Nanocrystals

Table S7. ICP–MS Elemental Analyses of Yb:Er:BaFBr Nanocrystals

Nominal		Experimental				
Yb + Er (mol. %)	Yb / Er	Yb + Er (mol. %)	Yb (mol. %)	Er (mol. %)	Yb / Er	100 × Er / (Yb + Er)
0.50	9.0	0.428	0.406	0.022	18.3	5.2
1.5	9.0	1.185	1.073	0.112	9.6	9.5
3.0	9.0	2.140	1.983	0.157	12.6	7.3
4.5	9.0	3.931	3.599	0.332	10.9	8.4
6.0	9.0	4.511	4.135	0.376	11.0	8.3

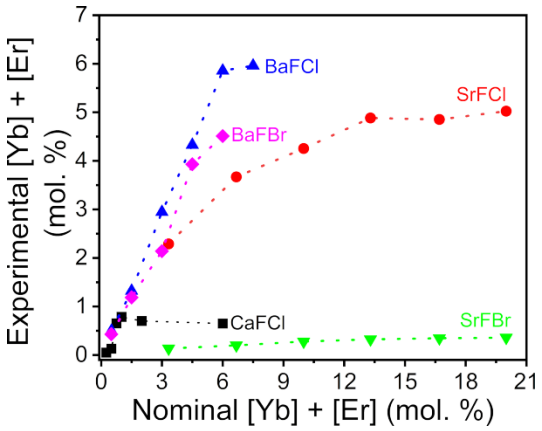

Figure S5. Metal concentration curves for Yb:Er:MFX nanocrystals (M = Ca, Sr, Ba; X = Cl, Br). Concentration curves show elemental analysis data from *Chem. Mater.* 2018, **30**, 2453, *Chem. Mater.* 2019, **31**, 6262, *J. Lumin.* 2021, **235**, 117974, and this work. Dotted lines are guides-to-the-eye.

6. Luminescence of Yb:Er:BaFBr Nanocrystals

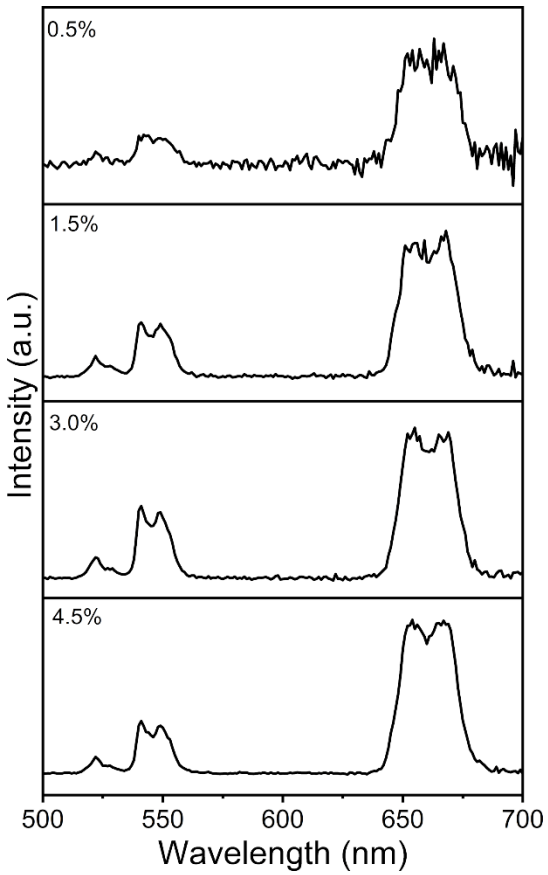

Figure S6. Steady-state emission spectra of Yb:Er:BaFBr nanocrystals under 980 nm excitation. Nominal total rare-earth concentrations are indicated.

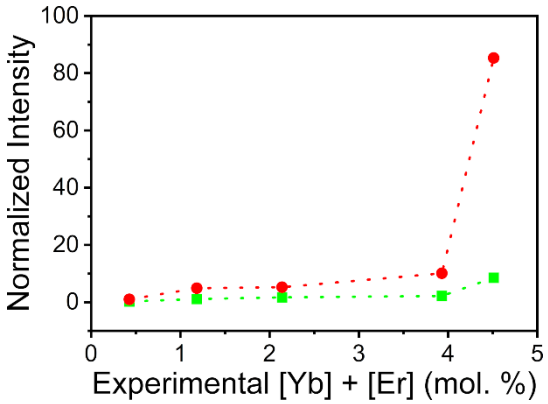

Figure S7. Integrated intensities of green (525 and 545 nm) and red emission bands (660 nm) as a function of the experimental total rare-earth concentration. Intensity values are normalized relative to the red band of the sample doped with ≈0.5 mol. %.

Table S8. Repeatability, Mean Calculated Temperature, and Temperature Resolution of Yb:Er:BaFBr Nanocrystals (6.0 mol. %)

Cycle #	175 K		300 K		400 K	
	$R(T)$	$T_{calculated}$ (K)	$R(T)$	$T_{calculated}$ (K)	$R(T)$	$T_{calculated}$ (K)
1	0.03003	185.3	0.20040	299.4	0.46976	393.5
2	0.02452	175.5	0.19932	299.0	0.46597	392.3
3	0.02559	177.6	0.19826	298.5	0.46206	391.1
4	0.02729	180.7	0.20590	301.7	0.46101	390.8
5	0.02662	179.5	0.20327	300.6	0.4714	394.0
6	0.02603	178.4	0.20894	303.0	0.47435	394.9
7	0.02738	180.9	0.20591	301.8	0.47652	395.5
8	0.02723	180.6	0.20658	302.0	0.47559	395.2
9	0.02802	182.0	0.20496	301.4	0.47638	395.5
10	0.02760	181.3	0.20625	301.9	0.46630	392.4
$\langle R(T) \rangle$	0.02703		0.20398		0.46993	
$\langle T_{calculated} \rangle$		180.2		300.9		393.5
ΔT		2.6		1.5		1.8