

Electron diffraction of ABX₃ perovskites with both the layered ordering of A-cations and the tilting of BX₆ octahedra

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Atomic positions and unit-cell descriptions for all space groups of ABX₃ perovskites with both the tilting of BX₆ octahedra and the layered ordering of A-cations. Note: The atomic coordinates for some Wyckoff positions are set exactly equal to special values, indicating that the Wyckoff positions should take the special atomic coordinate if BX₆ octahedra are perfectly rigid without distortion.

Tilt system number	Extended Glazer notation	Space group	Wyckoff positions			
			A cation (layer 1)	A cation (layer 2)	B cation	X anion
1-1	$A^+b^+c^+$	<i>Pmmm</i> (#47) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx 2a_p$	(1a) 0, 0, 0 (1c) 0, 0, 1/2 (1e) 0, 1/2, 0 (1g) 0, 1/2, 1/2	(1b) 1/2, 0, 0 (1d) 1/2, 0, 1/2 (1f) 1/2, 1/2, 0 (1h) 1/2, 1/2, 1/2	(8a) x, y, z $= 1/4, 1/4, 1/4$	(4u) 0, y_1, z_1 $y_1, z_1 \approx 1/4, 1/4$ (4v) 1/2, y_2, z_2 $y_2, z_2 = y_1+1/2, z_1+1/2$ (4w) $x_3, 0, z_3$ $x_3, z_3 \approx 1/4, 1/4$ (4x) $x_4, 1/2, z_4$ $x_4, z_4 = x_3+1/2, z_3+1/2$ (4y) $x_5, y_5, 0$ $x_5, y_5 \approx 1/4, 1/4$ (4z) $x_6, y_6, 1/2$ $x_6, y_6 = x_5+1/2, y_5+1/2$
4-1	$A^+b^+c^-$	<i>Pmm2</i> (#25) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx 2a_p$	(1a) 0, 0, z $z \approx 1/4$ (1a) 0, 0, z $z \approx 3/4$ (1b) 0, 1/2, z $z \approx 1/4$ (1b) 0, 1/2, z $z \approx 3/4$	(1c) 1/2, 0, z $z \approx 1/4$ (1c) 1/2, 0, z $z \approx 3/4$ (1d) 1/2, 1/2, z $z \approx 1/4$ (1d) 1/2, 1/2, z $z \approx 3/4$	(4i) x, y, z $= 1/4, 1/4, 0$ (4i) x, y, z $= 1/4, 1/4, 1/2$	(2e) $x_1, 0, z_1$ $x_1, z_1 \approx 1/4, 0$ (2e) $x_2, 0, z_2$ $x_2, z_2 \approx 1/4, 1/2$ (2f) $x_3, 1/2, z_3$ $x_3, z_3 = x_1+1/2, -z_1$ (2f) $x_4, 1/2, z_4$ $x_4, z_4 = x_2+1/2, -z_2$ (2g) 0, y_5, z_5 $y_5, z_5 \approx 1/4, 0$ (2g) 0, y_6, z_6 $y_6, z_6 \approx 1/4, 1/2$ (2h) 1/2, y_7, z_7 $y_7, z_7 = y_5+1/2, -z_5$ (2h) 1/2, y_8, z_8 $y_8, z_8 = y_6+1/2, -z_6$ (4i) x_9, y_9, z_9 $\approx 1/4, 1/4, 1/4$ (4i) x_{10}, y_{10}, z_{10} $= x_9+1/2, y_9+1/2, -z_9$
4-2	$a^+b^+C^-$	<i>Pmm2</i> (#25) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx 2a_p$	(1a) 0, 0, z $z \approx 1/4$ (1b) 0, 1/2, z $z \approx 1/4$ (1c) 1/2, 0, z $z \approx 1/4$ (1d) 1/2, 1/2, z	(1a) 0, 0, z $z \approx 3/4$ (1b) 0, 1/2, z $z \approx 3/4$ (1c) 1/2, 0, z $z \approx 3/4$ (1d) 1/2, 1/2, z	(4i) x, y, z $= 1/4, 1/4, 0$ (4i) x, y, z $= 1/4, 1/4, 1/2$	(2e) $x_1, 0, z_1$ $x_1, z_1 \approx 1/4, 0$ (2e) $x_2, 0, z_2$ $x_2, z_2 \approx 1/4, 1/2$ (2f) $x_3, 1/2, z_3$ $x_3, z_3 = x_1+1/2, -z_1$ (2f) $x_4, 1/2, z_4$

			$z \approx 1/4$	$z \approx 3/4$		$x_4, z_4 = x_2 + 1/2, -z_2$ (2g) $0, y_5, z_5$ $y_5, z_5 \approx 1/4, 0$ (2g) $0, y_6, z_6$ $y_6, z_6 \approx 1/4, 1/2$ (2h) $1/2, y_7, z_7$ $y_7, z_7 = y_5 + 1/2, -z_5$ (2h) $1/2, y_8, z_8$ $y_8, z_8 = y_6 + 1/2, -z_6$ (4i) x_9, y_9, z_9 $\approx 1/4, 1/4, 1/4$ (4i) x_{10}, y_{10}, z_{10} $= x_9 + 1/2, y_9 + 1/2, -z_9$
5-1	$a^+ a^+ c^-$	$P\bar{4}m2$ (#115) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx 2a_p$	(1a) $0, 0, 0$ (1b) $1/2, 1/2, 0$ (2g) $0, 1/2, z$ $z \approx 0$	(1c) $1/2, 1/2, 1/2$ (1d) $0, 0, 1/2$ (2g) $0, 1/2, z$ $z \approx 1/2$	(8l) x, y, z $= 1/4, 1/4, 1/4$	(4h) $x_1, x_1, 0$ $x_1 \approx 1/4$ (4i) $x_2, x_2, 1/2$ $x_2 = x_1 + 1/2$ (4j) $x_3, 0, z_3$ $x_3, z_3 \approx 1/4, 1/4$ (4j) $x_4, 0, z_4$ $x_4, z_4 \approx 1/4, 3/4$ (4k) $x_5, 1/2, z_5$ $x_5, z_5 = x_3 + 1/2, -z_3 + 1/2$ (4k) $x_6, 1/2, z_6$ $x_6, z_6 = x_4 + 1/2, -z_4 + 1/2$
8-1	$a^- b^+ c^-$	Pm (#6:b) $a \approx 2^{1/2} a_p$ $b \approx 2a_p$ $c \approx 2^{1/2} a_p$ $\beta \neq 90^\circ$	(1a) $x, 0, z$ $x, z \approx 0, 0$ (1a) $x, 0, z$ $x, z \approx 1/2, 1/2$	(1b) $x, 1/2, z$ $x, z \approx 0, 0$ (1b) $x, 1/2, z$ $x, z \approx 1/2, 1/2$	(2c) x, y, z $= 1/2, 1/4, 0$ (2c) x, y, z $= 0, 1/4, 1/2$	(1a) $x_1, 0, z_1$ $x_1, z_1 \approx 0, 1/2$ (1a) $x_2, 0, z_2$ $x_2, z_2 \approx 1/2, 0$ (1b) $x_3, 1/2, z_3$ $x_3, z_3 = -x_1, -z_1$ (1b) $x_4, 1/2, z_4$ $x_4, z_4 = -x_2, -z_2$ (2c) x_3, y_3, z_3 $\approx 1/4, 1/4, 1/4$ (2c) x_4, y_4, z_4 $= -x_3, y_3 + 1/2, -z_3$ (2c) x_5, y_5, z_5 $\approx 1/4, 3/4, 3/4$ (2c) x_6, y_6, z_6 $= -x_5, y_5 + 1/2, -z_5$
8-2	$A^- b^+ c^-$	$P2_1/m$ (#11:b) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx 2a_p$ $\beta \neq 90^\circ$	(2e) $x, 1/4, z$ $x, z \approx 0, 0$ (2e) $x, 1/4, z$ $x, z \approx 0, 1/2$	(2e) $x, 1/4, z$ $x, z \approx 1/2, 0$ (2e) $x, 1/4, z$ $x, z \approx 1/2, 1/2$	(4f) x, y, z $= 1/4, 0, 1/4$ (4f) x, y, z $= 3/4, 0, 1/4$	(2e) $x_1, 1/4, z_1$ $x_1, z_1 \approx 1/4, 1/4$ (2e) $x_2, 1/4, z_2$ $x_2, z_2 = -x_1 + 1/2, -z_1$ (2e) $x_3, 1/4, z_3$ $x_3, z_3 \approx 3/4, 1/4$ (2e) $x_4, 1/4, z_4$ $x_4, z_4 = -x_3 + 1/2, -z_3$ (4f) x_5, y_5, z_5 $\approx 0, 0, 1/4$ (4f) x_6, y_6, z_6 $= -x_5 + 1/2, -y_5, -z_5 + 1/2$ (4f) x_7, y_7, z_7 $\approx 1/4, 0, 0$ (4f) x_8, y_8, z_8 $= -x_7 + 1/2, -y_7, -z_7 + 1/2$

10-1	$A^+b^-b^-$	$Pmc2_1$ (#26) $a \approx 2a_p$ $b \approx 2^{1/2}a_p$ $c \approx 2^{1/2}a_p$	(2a) 0, y, z $y, z \approx 1/4, 1/2$	(2b) 1/2, y, z $y, z \approx 1/4, 1/2$	(4c) x, y, z $= 3/4, 3/4, 1/2$	(2a) 0, y_1, z_1 $y_1, z_1 \approx 1/4, 0$ (2b) 1/2, y_2, z_2 $y_2, z_2 = -y_1+1/2, -z_1$ (4c) x_3, y_3, z_3 $\approx 3/4, 0, 1/4$ (4c) x_4, y_4, z_4 $= -x_3+1/2, y_3+1/2, -z_3+1/2$
12-1	$a^-b^-C^-$	$C\bar{1}$ (#2) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx 2a_p$	(4i) x, y, z $\approx 1/4, 0, 0$	(4i) x, y, z $\approx 1/4, 0, 1/2$	(4i) x, y, z $= 0, 1/4, 1/4$ (4i) x, y, z $= 0, 1/4, 3/4$	(4i) x_1, y_1, z_1 $x_1 = 1/4, y_1 \approx 1/4, z_1 \approx 1/4$ (4i) x_2, y_2, z_2 $= x_1, y_1+1/2, z_1+1/2$ (4i) x_3, y_3, z_3 $x_3 \approx 1/2, y_3 = 1/2, z_3 \approx 1/4$ (4i) x_4, y_4, z_4 $= x_3+1/2, y_3, z_3+1/2$ (4i) x_5, y_5, z_5 $x_5 \approx 0, y_5 \approx 1/4, z_5 = 1/2$ (4i) x_6, y_6, z_6 $= x_5, y_5+1/2, z_5+1/2$
13-1	$A^-b^-b^-$	$P2/c$ (#13:b1) $a \approx 2a_p$ $b \approx 2^{1/2}a_p$ $c \approx 2^{1/2}a_p$ $\beta \neq 90^\circ$	(2e) 0, y, 1/4 $y \approx 1/4$	(2f) 1/2, y, 1/4 $y \approx 1/4$	(4g) x, y, z $= 1/4, 3/4, 1/4$	(2e) 0, $y_1, 1/4$ $y_1 \approx 3/4$ (2f) 1/2, $y_2, 1/4$ $y_2 = -y_1+1/2$ (4g) x_3, y_3, z_3 $\approx 1/4, 0, 0$ (4g) x_4, y_4, z_4 $= x_3+1/2, y_3+1/2, z_3+1/2$
16-1	$a^+a^+C^0$	$P4/mmm$ (#123) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx 2a_p$	(1a) 0, 0, 0 (1c) 1/2, 1/2, 0 (2f) 0, 1/2, 0	(1b) 0, 0, 1/2 (1d) 1/2, 1/2, 1/2 (2e) 1/2, 0, 1/2	(8r) x, x, z $x, z = 1/4, 1/4$	(4j) $x_1, x_1, 0$ $x_1 \approx 1/4$ (4k) $x_2, x_2, 1/2$ $x_2 = x_1+1/2$ (8s) $x_3, 0, z_3$ $x_3 = 1/4, z_3 \approx 1/4$ (8t) $x_4, 1/2, z_4$ $x_4, z_4 = x_3+1/2, z_3+1/2$
17-1	$a^+B^0c^-$	$Pmma$ (#51) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx 2a_p$	(2e) 1/4, 0, z $z \approx 0$ (2e) 1/4, 0, z $z \approx 1/2$	(2f) 1/4, 1/2, z $z \approx 0$ (2f) 1/4, 1/2, z $z \approx 1/2$	(8l) x, y, z $= 1/2, 1/4, 1/4$	(4g) 0, $y_1, 0$ $y_1 \approx 1/4$ (4h) 0, $y_2, 1/2$ $y_2 = y_1+1/2$ (4i) $x_3, 0, z_3$ $x_3, z_3 \approx 0, 1/4$ (4j) $x_4, 1/2, z_4$ $x_4, z_4 = x_3, z_3+1/2$ (4k) 1/4, y_5, z_5 $y_5, z_5 \approx 1/4, 1/4$ (4k) 1/4, y_6, z_6 $y_6, z_6 = y_5+1/2, z_5+1/2$
17-2	$A^+b^0c^-$	$Amm2$ (#38) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx 2a_p$	(2e) 1/4, 0, z $z \approx 0$ (2e) 1/4, 0, z $z \approx 1/2$	(2f) 1/4, 1/2, z $z \approx 0$ (2f) 1/4, 1/2, z $z \approx 1/2$	(8l) x, y, z $= 1/2, 1/4, 1/4$	(4c) $x_1, 0, z_1$ $x_1, z_1 \approx 1/4, 1/4$ (4c) $x_2, 0, z_2$ $x_2, z_2 = -x_1+1/2, -z_1$ (4d) 0, y_3, z_3 $y_3, z_3 \approx 1/4, 1/4$ (4e) 0, y_4, z_4 $y_4, z_4 = -y_3+1/2, z_3$ (8f) x_5, y_5, z_5 $\approx 3/4, 1/4, 0$

17-3	$a^+b^0c^-$	<i>Pmma</i> (#51) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx 2a_p$	(2e) $1/4, 0, z$ $z \approx 0$ (2f) $1/4, 1/2, z$ $z \approx 0$	(2e) $1/4, 0, z$ $z \approx 1/2$ (2f) $1/4, 1/2, z$ $z \approx 1/2$	(8l) x, y, z $= 1/2, 1/4, 1/4$	(4g) $0, y_1, 0$ $y_1 \approx 1/4$ (4h) $0, y_2, 1/2$ $y_2 = y_1 + 1/2$ (4i) $x_3, 0, z_3$ $x_3, z_3 \approx 0, 1/4$ (4j) $x_4, 1/2, z_4$ $x_4, z_4 = x_3, z_3 + 1/2$ (4k) $1/4, y_5, z_5$ $y_5, z_5 \approx 1/4, 1/4$ (4k) $1/4, y_6, z_6$ $y_6, z_6 = y_5 + 1/2, z_5 + 1/2$
19-1	$a^-B^0c^-$	<i>P2/m</i> (#10:b) $a \approx 2^{1/2}a_p$ $b \approx 2a_p$ $c \approx 2^{1/2}a_p$ $\beta \neq 90^\circ$	(2m) $x, 0, z$ $x, z \approx 1/4, 3/4$	(2n) $x, 1/2, z$ $x, z \approx 1/4, 3/4$	(4o) x, y, z $= 1/4, 1/4, 1/4$	(2i) $0, y_1, 0$ $y_1 \approx 1/4$ (2j) $1/2, y_2, 0$ $y_2 \approx 1/4$ (2k) $0, y_3, 1/2$ $y_3 = y_2 + 1/2$ (2l) $1/2, y_4, 1/2$ $y_4 = y_1 + 1/2$ (2m) $x_5, 0, z_5$ $x_5, z_5 \approx 1/4, 1/4$ (2n) $x_6, 1/2, z_6$ $x_6, z_6 = x_5 + 1/2, z_5 + 1/2$
19-2	$A^-b^0c^-$	<i>A2/m</i> (#12:b2) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx 2a_p$ $\beta \neq 90^\circ$	(4i) $x, 0, z$ $x = 0, z \approx 1/4$	(4i) $x, 0, z$ $x = 1/2, z \approx 1/4$	(8j) x, y, z $= 1/4, 1/4, 0$	(4g) $0, y_1, 0$ $y_1 \approx 1/4$ (4h) $1/2, y_2, 1/2$ $y_2 = y_1$ (4i) $x_3, 0, z_3$ $x_3, z_3 \approx 1/4, 0$ (4i) $x_4, 0, z_4$ $x_4, z_4 = -x_3 + 1/2, -z_3 + 1/2$ (8j) x_5, y_5, z_5 $x_5, z_5 = 1/4, 1/4, y_5 \approx 1/4$
20-1	$a^-B^0a^-$	<i>Pmma</i> (#51) $a \approx 2^{1/2}a_p$ $b \approx 2a_p$ $c \approx 2^{1/2}a_p$	(2e) $1/4, 0, z$ $z \approx 1/4$	(2f) $1/4, 1/2, z$ $z \approx 1/4$	(4k) $1/4, y, z$ $y, z = 1/4, 3/4$	(2e) $1/4, 0, z_1$ $z_1 \approx 3/4$ (2f) $1/4, 1/2, z_2$ $z_2 = -z_1 + 1/2$ (4g) $0, y_3, 0$ $y_3 \approx 1/4$ (4h) $0, y_4, 1/2$ $y_4 = -y_3 + 1/2$
21-1	$A^0b^0c^+$	<i>Pmmm</i> (#47) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx a_p$	(1c) $0, 0, 1/2$ (1g) $0, 1/2, 1/2$	(1d) $1/2, 0, 1/2$ (1h) $1/2, 1/2, 1/2$	(4y) $x, y, 0$ $x, y = 1/4, 3/4$	(2i) $x_1, 0, 0$ $x_1 \approx 1/4$ (2k) $x_2, 1/2, 0$ $x_2 = x_1 + 1/2$ (2m) $0, y_3, 0$ $y_3 \approx 1/4$ (2o) $1/2, y_4, 0$ $y_4 = y_3 + 1/2$ (4z) $x_5, y_5, 1/2$ $x_5, y_5 = 1/4, 1/4$
21-2	$a^0a^0c^+$	<i>P4/mbm</i> (#127) $a \approx 2^{1/2}a_p$ $b \approx 2^{1/2}a_p$ $c \approx 2a_p$	(2c) $1/2, 0, 1/2$	(2d) $0, 1/2, 0$	(4e) $0, 0, z$ $z = 1/4$	(2a) $0, 0, 0$ (2b) $1/2, 1/2, 1/2$ (8k) $x, x + 1/2, z$ $x \approx 1/4, z = 1/4$
22-1	$a^0b^-C^0$	<i>Cmmm</i> (#65) $a \approx 2a_p$ $b \approx 2a_p$ $c \approx 2a_p$	(4i) $0, y, 0$ $y \approx 1/4$	(4j) $0, y, 1/2$ $y \approx 1/4$	(8o) $x, 0, z$ $x, z = 1/4, 1/4$	(4g) $x_1, 0, 0$ $x_1 \approx 1/4$ (4h) $x_2, 0, 1/2$ $x_2 = -x_1 + 1/2$ (4k) $0, 0, z_3$

						$z_3 \approx 1/4$ $(4l) 1/2, 0, z_4$ $z_4 = -z_3 + 1/2$ $(8m) 1/4, 1/4, z_5$ $z_5 \approx 1/4$
22-2	$a^0 a^0 C^-$	<i>P4/nbm</i> (#125:2) $a \approx 2^{1/2} a_p$ $b \approx 2^{1/2} a_p$ $c \approx 2a_p$	(2c) $3/4, 1/4, 0$	(2d) $3/4, 1/4, 1/2$	(4g) $3/4, 3/4, z$ $z = 1/4$	$(2a) 3/4, 3/4, 0$ $(2b) 3/4, 3/4, 1/2$ $(8m) x+1/2, x, z$ $x \approx 1/2, z = 1/4$
23-1	$a^0 a^0 C^0$	<i>P4/mmm</i> (#123) $a = a_p$ $b = a_p$ $c = 2a_p$	(1c) $1/2, 1/2, 0$	(1d) $1/2, 1/2, 1/2$	(2g) $0, 0, z$ $z = 1/4$	$(1a) 0, 0, 0$ $(1b) 0, 0, 1/2$ $(4i) 0, 1/2, z$ $z = 1/4$