## Supporting Information

# A New Organic-Inorganic Hybrid Perovskite Ferroelectric $[ClCH_2CH_2N(CH_3)_3][PbBr_3]$ and Its PVDF Matrix-assisted Highly-oriented Flexible Ferroelectric Films

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### Calculation of the polarization of CEPbBr with a point charge model

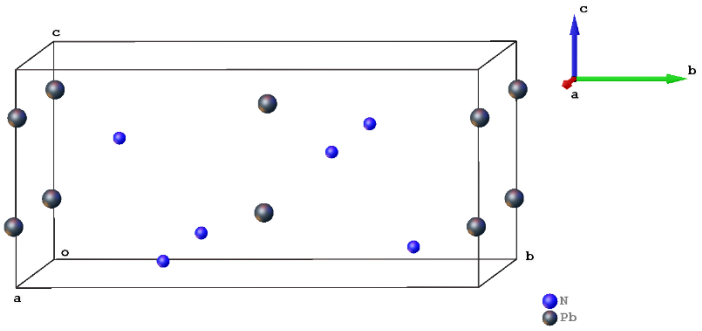


**Figure S1.** Atoms distribution of low-temperature phase of **CEPbBr** at 223 K for the calculation of polarization with a point charge model.

According to the crystal structure data collected at 223 K, we select a unit cell and make an assumption that the positive charge of $[ClCH_2CH_2N(CH_3)_3]^+$ and the negative charge of $[PbBr_3]^-$ is on the N atom and Pb atom, respectively.

| Atoms | Coordinate | | | Center coordinate |
|---|---|---|---|---|
| Pb | 0.5 | 0.5 | 0.28 | (0.5,0.5,0.53) |
| Pb | 1 | 1 | 0.78 | |
| Pb | 1 | 0 | 0.28 | |
| Pb | 0 | 1 | 0.28 | |
| Pb | 0 | 0 | 0.28 | |
| Pb | 1 | 1 | 0.28 | |

| | | | | |
|---|---|---|---|---|
| Pb | 1 | 0 | 0.78 | |
| Pb | 0 | 0 | 0.78 | |
| Pb | 0.5 | 0.5 | 0.78 | |
| Pb | 0 | 1 | 0.78 | |
| N | 0.5 | 0.182 | 0.62 | (0.5,0.5,0.37) |
| N | 0 | 0.318 | 0.12 | |
| N | 0 | 0.682 | 0.62 | |
| N | 1 | 0.682 | 0.62 | |
| N | 0.5 | 0.818 | 0.12 | |
| N | 1 | 0.318 | 0.12 | |

According to the center coordinate, the polarization can only be calculated along *c* axis, it does not exist along *a* or *b* axis.

$P_S = lim\frac{1}{V}\sum q_i r_i$

$= (q_{Pb}r_{Pb} + q_N r_N) / V$

$= [(-e\times0.53)+ (e\times0.37)]\times4\times c/V$

$= [-0.16\times4\times1.6 \times 10^{-19} \times8.747 \times 10^{-10}\ C\ m] / (1259 \times 10^{-30}\ m^3)$

$= -6.6\times10^{-2} C\ m^{-2}$

$|Ps| = 6.6\ \mu C\ cm^{-2}$

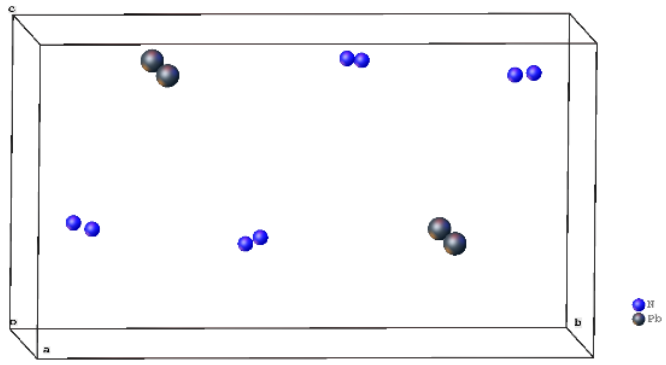


**Figure S2.** Atoms distribution of high-temperature phase of **CEPbBr** at 340 K for the calculation of polarization with a point charge model.

According to the crystal structure data collected at 340 K, we select a unit cell and

make an assumption that the positive charge of $[ClCH_2CH_2N(CH_3)_3]^+$ and the negative charge of $[PbBr_3]^-$ is on the N atom and Pb atom, respectively.

| Atoms | Coordinate | | | Center coordinate |
|---|---|---|---|---|
| N | 0.636 | 0.906 | 0.871 | (0.5,0.5,0.6145) |
| N | 0.136 | 0.594 | 0.871 | |
| N | 0.864 | 0.406 | 0.371 | |
| N | 0.562 | 0.876 | 0.858 | |
| N | 0.062 | 0.624 | 0.858 | |
| N | 0.364 | 0.094 | 0.371 | |
| N | 0.938 | 0.376 | 0.358 | |
| N | 0.438 | 0.124 | 0.358 | |
| Pb | 0.055 | 0.248 | 0.857 | (0.5,0.5,0.607) |
| Pb | 0.555 | 0.252 | 0.857 | |
| Pb | 0.445 | 0.748 | 0.357 | |
| Pb | 0.945 | 0.752 | 0.357 | |

According to the center coordinate, the polarization can only be calculated along *c* axis, it does not exist along *a* or *b* axis.

$$P_S = lim\frac{1}{V}\sum q_i r_i$$

$= (q_{Pb}r_{Pb} + q_N r_N) / V$

$= [(-e\times0.607)+ (e\times0.6145)]\times2\times c/V$

$= [0.0075\times2\times1.6 \times 10^{-19} \times9.7334\times 10^{-10}\ C\ m] / (1330.500 \times 10^{-30}\ m^3)$

$= 1.756\times10^{-3} C\ m^{-2}$

$|Ps| = 0.1756 \mu C\ cm^{-2}$