Supplementary information

Lead-Free Double Perovskites $Cs_2InCuCl_6$ and $(CH_3NH_3)_2InCuCl_6$: Electronic, Optical, and Electrical Properties

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Table of Contents

S1. Computational details for c-Si, CdTe

The PBEsol functional and a kinetic energy cutoff of 500 eV were employed to optimize the structures of c-Si and CdTe. A k-mesh of 14 × 14 × 14 and 12 × 12 × 12 were used to sample the first Brillouin zone for c-Si and CdTe, respectively. For the HSE06-SOC band gap calculation, a k-mesh of 8 × 8 × 8 was used for both materials. The absorption coefficient is computed using the procedure described in the **Computational Methods** section of the main text.

S2. Goldschmidt's empirical criteria

For a perovskite ABX_3, the Goldschmidt tolerance factor is calculated using

$$\boldsymbol{t} = \frac{(\boldsymbol{R_A} + \boldsymbol{R_X})}{\sqrt{\boldsymbol{2}}(\boldsymbol{R_B} + \boldsymbol{R_X})} \quad (1)$$

The octahedral factor is calculated using

$$\boldsymbol{\mu} = \frac{\boldsymbol{R_B}}{\boldsymbol{R_X}} \quad (2)$$

where R_A, R_B, R_X are the radius of A, B, and X, respectively. We use the Shannon radii (reference: v.web.umkc.edu/vanhornj/Radii.xls) as given in Table S1. For double perovskites, the radius for B site is computed by taking the average of the two metals.

Table S1. Shannon radii (in Å) used in this work.

	Cs (VIII)	In (VI)	Cu (VI)	Ag (VI)	Au (VI)	Cl (VI)	Br (VI)	I (VI)
Radius	1.88	0.8	0.77	1.15	1.37	1.81	1.96	2.2

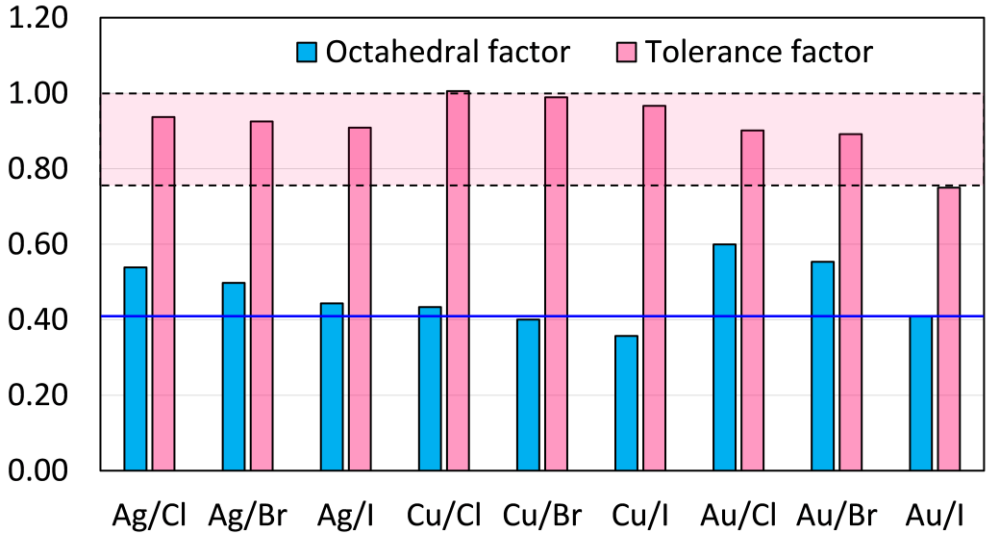

Figure S1. Octahedral (μ) and tolerance factors (t) for Cs_2InMX_6 structure (M = Cu, Ag, Au and X = Cl, Br, I). The blue line at 0.41 indicates the lower bound of μ and the pink region indicates the optimal range of t ($0.75 \leq t \leq 1.00$) for a stable perovskite structure.

S3. Total electronic energies used in the decomposition enthalpy calculations

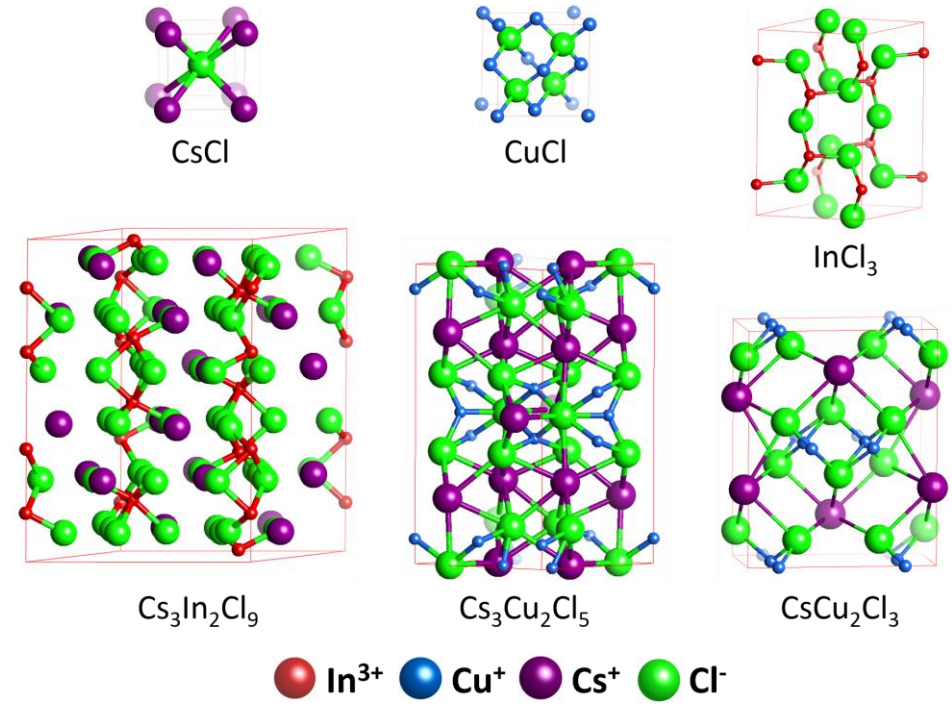

Figure S2. Crystal structures for the compounds used in the decomposition calculation.

Table S2. Total electronic energies used in the decomposition enthalpy calculations.

Compound	Total energy per formula unit (eV)
CsCl	-6.8526
CuCl	-7.0648
$InCl_3$	-13.4231
$CsCu_2Cl_3$	-21.3152
$Cs_3Cu_2Cl_5$	-35.2731
$Cs_3In_2Cl_9$	-48.7434
$Cs_2InCuCl_6$	-34.8672

S4. Indirect and direct band gap for $Cs_2InCuCl_6$ and $(MA)_2InCuCl_6$

Table S3. Calculated band gap for $Cs_2InCuCl_6$ and $(MA)_2InCuCl_6$.

	HSE06-SOC		PBE0-SOC	
	Direct gap	Indirect gap	Direct gap	Indirect gap
$Cs_2InCuCl_6$	1.054	NA	1.732	NA
$(MA)_2InCuCl_6$ (HA)	1.527	1.312	2.188	1.980
$(MA)_2InCuCl_6$ (HB)	1.738	1.427	2.394	2.090

S5. Absolute band edge position calculations

The slab model of $Cs_2InCuCl_6$ is constructed using a 1 × 1 × 2 supercell of the conventional cell. These layers are separated by 25 Å thick vacuum region along the z direction. This thickness is sufficient since the planar average of the electrostatic potential along the z-axis is converged as shown in Figure S2.

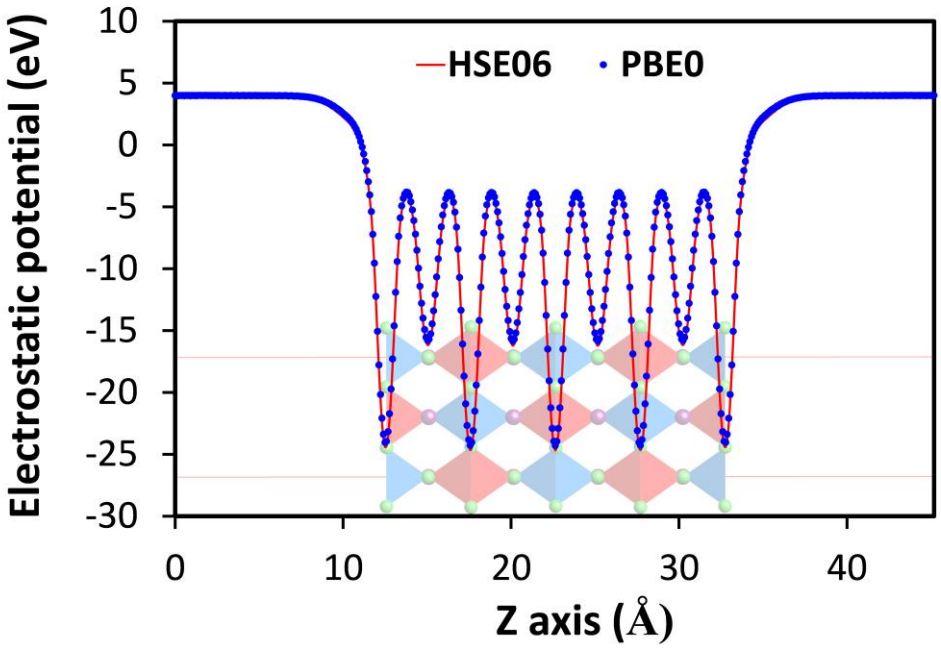

Figure S3. The planar average of the electrostatic potential along the z-axis computed by HSE06 and PBE0 functional.

The absolute valence band maximum (E_{VBM}) is computed using

$$\mathbf{E_{VBM} = -\Phi = \varepsilon_F - E_{vacuum}} \quad (3)$$

where Φ is the work function, ε_F is Fermi level, E_{vacuum} is the electrostatic potential of the vacuum.

S6. Optical absorption coefficient calculations

The complex index of refraction $\mathrm{k}_{\alpha\alpha}(\omega)$ is given by

$$\mathbf{k}_{\alpha\alpha}(\boldsymbol{\omega}) = \sqrt{\frac{|\boldsymbol{\epsilon}_{\alpha\alpha}(\boldsymbol{\omega})| - \mathbf{Re}\boldsymbol{\epsilon}_{\alpha\alpha}(\boldsymbol{\omega})}{\mathbf{2}}} \tag{4}$$

where ω is the frequency, $\epsilon_{\alpha\alpha}(\omega)$ is the complex frequency-dependent dielectric tensor and $\mathrm{Re}\epsilon_{\alpha\alpha}(\omega)$ is its real part. $\epsilon_{\alpha\alpha}(\omega)$ is obtained by using the keyword LOPTICS = .TRUE. in the INCAR file.

Following, the absorption coefficient can be computed from

$$\mathbf{A}_{\alpha\alpha}(\boldsymbol{\omega}) = \frac{\mathbf{2}\boldsymbol{\omega}\mathbf{k}_{\alpha\alpha}(\boldsymbol{\omega})}{\boldsymbol{c}} \tag{5}$$

where c is the speed of light.

S7. Charge carrier mobility calculations

The elastic constant C is calculated by fitting the difference in total energy of the unit cell as a function of the dilation $\frac{\Delta l}{l_o}$.

$$\boldsymbol{\Delta E} = \boldsymbol{E} - \boldsymbol{E_o} = \frac{\mathbf{1}}{\mathbf{2}}\boldsymbol{V_o C} \times (\frac{\boldsymbol{\Delta l}}{\boldsymbol{l_o}})^{\mathbf{2}} \tag{6}$$

where E_o and V_o are the total energy and volume of the unit cell at the equilibrium, respectively.

The deformation potential constant E_1 is calculated using a similar approach. The band edge position (VBM or CBM) is also a function of the dilation $\frac{\Delta l}{l_o}$.

$$\boldsymbol{E^{Band\ edge}} = \boldsymbol{E_o^{Band\ edge}} + \boldsymbol{E_1} \times \frac{\boldsymbol{\Delta l}}{\boldsymbol{l_o}} \tag{7}$$

where the band edge is VBM or CBM for hole or electron, respectively. Details of these fittings are shown in Figure S3.

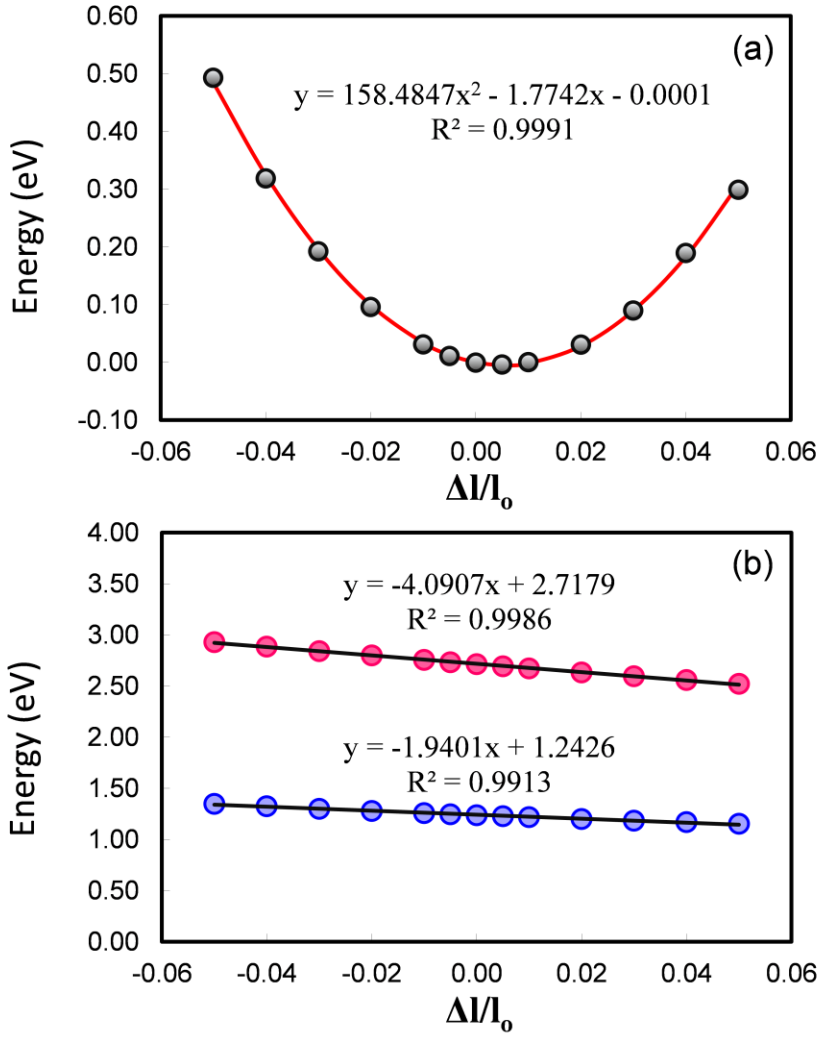

Figure S4. The energy-strain relationship (a) and the band edge positions (VBM in blue; CBM in pink) as a function of the dilation (b).

S8. Optimized crystal structures in VASP/POSCAR format

```
Cs2InCuCl6
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    7.1358944193499934   -0.0000000000053973   -0.0000000000038165
    3.5679472097151756    6.1798658458916060   -0.0000000000052134
    3.5679472097151752    2.0599552819888562    5.8264333952269407
  In   Cu   Cs   Cl
    1    1    2    6
Direct
```

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0.2500000000000000 0.2500000000000000 0.2500000000000000
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0.7541100912936539 0.2458899087063463 0.2458899087063463
0.7541100912936539 0.2458899087063463 0.7541100912936539
0.2458899087063463 0.7541100912936539 0.2458899087063463
0.7541100912936539 0.7541100912936539 0.2458899087063463
0.2458899087063463 0.2458899087063463 0.7541100912936539

Cs2InCuBr6

1.00000000000000

7.5328733926506946 -0.0000000000028476 -0.0000000000019499
3.7664366963702922 6.5236597215595786 -0.0000000000030622
3.7664366963755782 2.1745532405405243 6.1505653696248119

In Cu Cs Br

1 1 2 6

Direct

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0.0000000000000000 0.0000000000000000 0.0000000000000000
0.7500000000000000 0.7500000000000000 0.7500000000000000
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0.7560682624220831 0.7560682624220902 0.2439317375783006
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Cs2InCuI6

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4.0572654212964592 2.3424632831712522 6.6254866886798203

In Cu Cs I

1 1 2 6

Direct

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0.2500000000000000 0.2500000000000000 0.2500000000000000
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0.7578577095825788 0.2421422904174216 0.2421422904174216
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0.2421422904174216 0.7578577095825788 0.2421422904174216

0.7578577095825788 0.7578577095825788 0.2421422904174216
0.2421422904174216 0.2421422904174216 0.7578577095825788

Cs2InAgCl6

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In Ag Cs Cl
1 1 2 6
Direct
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Cs2InAgBr6

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In Ag Cs Br
1 1 2 6
Direct
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Cs2InAgI6

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```
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 0.0000000000000000  0.0000000000000000  0.0000000000000000
 0.7500000000000000  0.7500000000000000  0.7500000000000000
 0.2500000000000000  0.2500000000000000  0.2500000000000000
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 0.7504251995086900  0.2495748004920272  0.7504251995086904
 0.2495748004920271  0.7504251995086901  0.2495748004920272
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```

Cs2InAuCl6

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     3.6737354355479668    2.1210321426517376    5.9991848446106344
  In   Au   Cs   Cl
   1    1    2    6
Direct
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-0.0000000000000000  0.0000000000000000 -0.0000000000000000
 0.7500000000000000  0.7500000000000000  0.7500000000000000
 0.2500000000000000  0.2500000000000000  0.2500000000000000
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Cs2InAuBr6

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     3.8614548155095099    2.2294119772071008    6.3057293084188748
  In   Au   Cs   Br
   1    1    2    6
Direct
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 0.0000000000000000  0.0000000000000000  0.0000000000000000
 0.7500000000000000  0.7500000000000000  0.7500000000000000
 0.2500000000000000  0.2500000000000000  0.2500000000000000
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Cs2InAuI6

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0.7535641282598303 0.7535641282598303 0.2464358717401696
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MA2InCuCl6-HA

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MA2InCuCl6-HB

1.00000000000000

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In Cu Cl C H N
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CsCl

1.00000000000000

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-0.0000000000000000 4.0722308931700608 -0.0000000000000000
0.0000000000000000 -0.0000000000000000 4.0722308931700608
Cs Cl
1 1
Direct
-0.0000000000000000 0.0000000000000000 -0.0000000000000000
0.5000000000000000 0.5000000000000000 0.5000000000000000

CuCl
1.00000000000000
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0.0000000000000000 5.2727505150888936 -0.0000000000000000
-0.0000000000000000 0.0000000000000000 5.2727505150888927
Cl Cu
4 4
Direct
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0.7500000000000000 0.2500000000000000 0.7500000000000000
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Cl In
6 2
Direct
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Cl Cu Cs

6 4 2
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Cs3Cu2Cl5
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0.0000000000000000 10.3315005629203398 0.0000000000000000
0.0000000000000000 0.0000000000000000 12.8553420659348276
Cs Cu Cl
12 8 20
Direct
0.5377213586473752 0.5119479267233008 0.8205214250825746
0.4622786923526397 0.4880520282766997 0.1794785569174297
0.9622786923526254 0.0119479507233096 0.3205214250825826
0.0377213236473686 0.9880520732766992 0.6794785749174254
0.3980119827999352 0.7500000000000000 0.4521369560682976
0.0377213236473686 0.5119479267233008 0.6794785749174254
0.6019880422000717 0.2500000000000000 0.5478630439317090
0.4622786923526397 0.0119479507233096 0.1794785569174297
0.8980119077999312 0.7500000000000000 0.0478630529317137
0.9622786923526254 0.4880520282766997 0.3205214250825826
0.1019880292000728 0.2500000000000000 0.9521369200682880
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0.2623089670071612 0.2500000000000000 0.3636445245858880
0.2941967208819413 0.7500000000000000 0.0507311965249875
0.2376910329928317 0.7500000000000000 0.8636445595858718
0.7941967208819336 0.7500000000000000 0.4492688124749952
0.7376910579928232 0.7500000000000000 0.6363554404141282
0.7058032791180664 0.2500000000000000 0.9492688124750164
0.7623089420071768 0.2500000000000000 0.1363554664141219
0.2058032921180561 0.2500000000000000 0.5507311875249836
0.6777150905529790 0.2500000000000000 0.2945788695962501
0.8115308727765899 0.0662302152460676 0.0525000780348409
0.7982350624874367 0.2500000000000000 0.7905954533475089
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0.0306506570745558 0.7500000000000000 0.4896270656999673
0.7017649375125633 0.7500000000000000 0.2905953993474975
0.6884691272234101 0.5662302372460823 0.5525000920348347
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0.3115308727765753 0.4337697627539380 0.4474999079651581
0.4693493589254458 0.2500000000000000 0.9896270296999874
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0.3115308727765753 0.0662302152460676 0.4474999079651581
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Cs3In2Cl9

1.00000000000000

9.5028226862740599 0.0305891186115024 0.0277067412570891

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1.0704219974613942 0.9590327230991063 9.3936039594200835

Cl Cs In

18 6 4

Direct

0.2637220126454114 0.0878235133417592 0.9207601348295654
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0.9121764716582468 0.0792398631704337 0.7362780453545915
0.4121764766582451 0.2362780193545851 0.5792398391704324
0.5878235273417496 0.7637219876454077 0.4207601268295615
0.2362779873545895 0.5792398551704337 0.4121765016582437
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0.4037627170829011 0.0962372969170979 0.2500000040000003
0.5962372379170955 0.9037626820829050 0.7499999870000025
0.2499999879999990 0.4037626990828996 0.0962372969170982
0.7499999380000020 0.5962373049170975 0.9037626940829060
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0.9106572938373367 0.5893428091626611 0.2500000040000003
0.0893428301626677 0.4106572208373364 0.7499999870000025
0.2499999919999993 0.9106571388373417 0.5893428251626625
0.7500000089999972 0.0893428221626670 0.4106572158373324

0.5893428111626613	0.2500000040000003	0.9106571478373389
0.4106571918373375	0.7500000029999967	0.0893428241626672
0.1518543916203634	0.1518544036203680	0.1518543956203638
0.8481455723796308	0.8481456013796297	0.8481455953796292
0.3481456443796344	0.3481456103796315	0.3481456123796317
0.6518544076203675	0.6518543946203700	0.6518543786203687