

Supporting Information

Multi-objective solid electrolyte design of tetragonal and cubic inverse-perovskites for all-solid-state lithium-ion batteries by high-throughput DFT calculations and AI-driven methods

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Table S1. DFT-calculated electronic band gap energy (E_g) values of known inorganic solid electrolytes.

Compound	E_g / eV	DFT functional
Garnet $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ ¹	4.3	PBE
	5.8	HSE06
	6.4	G0W0
LISICON $\gamma\text{-Li}_3\text{PO}_4$ ²	5.7	LSDA
NASICON $\text{Li}_{1+x}\text{Al}_x\text{Ti}_{2-x}(\text{PO}_4)_3$ ($x = 0.17$) ³	2.4	PBE
Perovskite $\text{Li}_x\text{La}_{1-x}\text{TiO}_3$ ($x = 0.5$) ⁴	2.4-2.9	LDA+U
Li_3N ⁵	1.1	PBE
$\text{Li}_2\text{PO}_2\text{N}$ (LiPON) ⁶	6	LDA
Thio-LISICON $\gamma\text{-Li}_3\text{PS}_4$ ⁷	3.7	HSE06
$\text{Li}_{10}\text{GeP}_2\text{S}_{12}$ ⁸	3.6	HSE06
Li_3YCl_6 ⁹	6.02	HSE

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About MSD slope fitting procedure

AIMD calculation is well known to be highly-accurate in estimating statistical observables (e.g., bulk Li ion diffusivity) but it needs sufficiently long sampling time for the production run. In the present work, we performed slope fitting in the linear regime of the MSD plot to determine bulk diffusivity/conductivity data. The MSD slope fitting procedure can be explained as follows. At first, we are aware that the AIMD method can become very expensive computationally when performed in the context of large-scale material screening such as in the present work. Keeping this in mind, we first carefully analyzed the MSD trends with respect to MD sampling time and MD temperature before doing the multi-objective optimization task for DFT-calculated solid electrolyte properties. Our analysis revealed that 50 ps and 400 K, respectively, are reasonable choices that can enable us to access the ‘linear’ regime of the MSD plot. Meanwhile, we point out that the MSD calculation was performed by time-ensemble averaging (ergodicity), this means that the tail part of the MSD plot has a relatively larger error/fluctuation than the middle and earlier part, this is due to the inherently smaller ensemble size of ion displacement values at the MSD tail part. In addition, we recognize that the earlier part of the MSD plot contains the ballistic regime which is dominated by local vibrations and back-and-forth Li ion jumps that do not contribute to long-range ion transport, this results to the observed MSD nonlinearity in this regime. Therefore, we excluded portions of the earlier and tail part of the MSD plot for the MSD slope fitting. The two boundary points of the MD step range for the MSD slope fitting were determined based on whether the instantaneous slope $d(MSD)/dt$ changes significantly or not at those points. Examples of fitted MSD slopes that we performed are shown in the figure below (shown as dashed lines) for three representative inverse-perovskite compounds. As can be seen, the data points in the earlier and tail part of the MSD plot were excluded during MSD slope fitting.

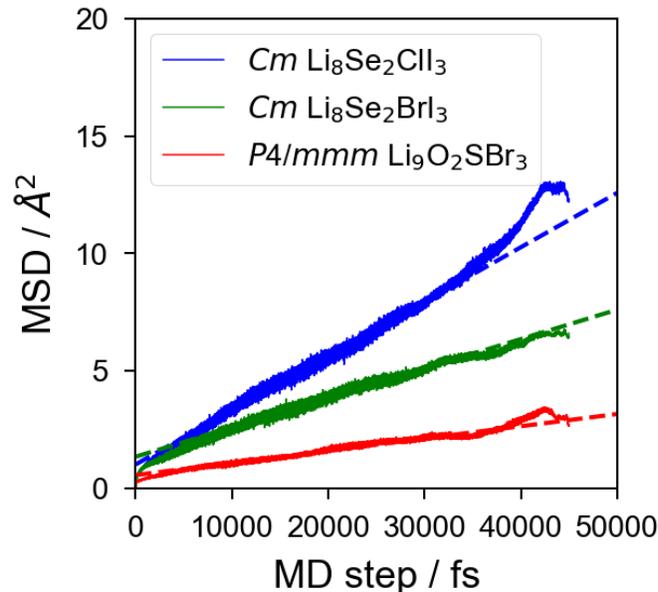


Figure S1. Mean square displacement (MSD) slope fitting for Li ions using the 50-ps AIMD trajectory data at 400 K for three representative Li-rich inverse-perovskite compounds. The dashed lines indicate the actual fitted MSD slope lines, with the two boundary points of the MD step range determined based on whether the instantaneous slope $d(MSD)/dt$ changes significantly or not at those points.

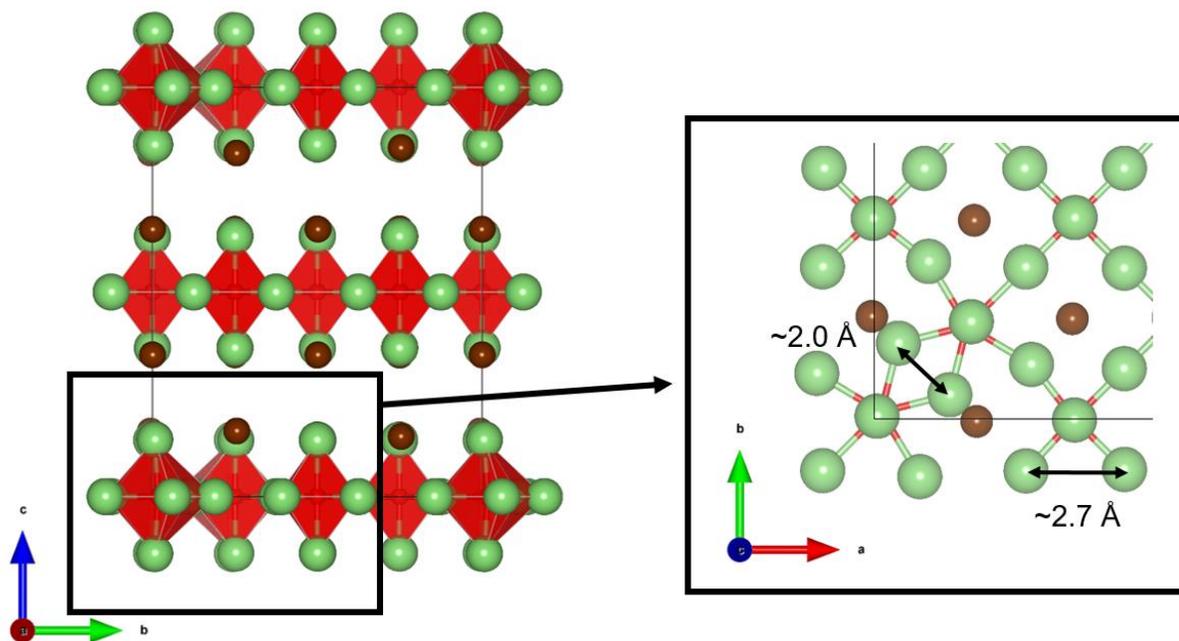


Figure S2. DFT-geometry-optimized structure of $I4/mmm$ Li_4OBr_2 antiperovskite compound with an added Li interstitial in one of the OLi_6 octahedral basal plane. The Li-Li nearest-neighbor distance with Li interstitial is $\sim 2.0 \text{ \AA}$, shorter than the regular Li-Li Wyckoff site interatomic distance which is $\sim 2.7 \text{ \AA}$.

Table S2. Summary list on region-1 compounds from Figure 9 of the main text.

Supercell formula	Space group	Base structure	Decomposition energy (E_d) / eV/atom	Crystal-likeness (CL) score
Li32Cl8O8F8	Cm	Li4XZ2	0.049	0.718
Li32I8Cl8O8	P4/mmm	Li4XZ2	0.029	0.504
Li24Se2I4Cl4O6	Ama2	Li3XZ	0.087	0.667
Li24Te2I2Br6O6	Pma2	Li3XZ	0.081	0.837
Li24Se4I6Br2O4	Pm	Li3XZ	0.087	0.578
Li16Se3I8O1	P4/mmm	Li4XZ2	0.098	0.754
Li16S3I6Cl2O1	P4mm	Li4XZ2	0.098	0.695
Li16S1I2Cl6O3	P4/mmm	Li4XZ2	0.081	0.529
Li14I4Br2O4	I4mm	Li7X2Z3	0.044	0.677
Li16S3I6Cl2O1	P4mm	Li4XZ2	0.097	0.516
Li24S2I4Br4O6	P4mm	Li3XZ	0.058	0.783
Li24S4I6Cl2O4	P4mm	Li3XZ	0.099	0.58
Li24Se2Br6Cl2O6	Pmm2	Li3XZ	0.069	0.726
Li24Se2S6I8	P4/mmm	Li3XZ	0.077	0.583
Li16S1I2Br6O3	P4mm	Li4XZ2	0.052	0.741
Li16S1I2Cl6O3	P4mm	Li4XZ2	0.068	0.611
Li16S4I2Br6	P4/nmm	Li4XZ2	0.092	0.518
Li32Se2I16O6	Cmcm	Li4XZ2	0.041	0.525
Li16Te1Br2Cl6O3	P4mm	Li4XZ2	0.093	0.587
Li24S2Cl6O6F2	Cmmm	Li3XZ	0.09	0.761
Li16Cl4O4F4	P4mm	Li4XZ2	0.096	0.807
Li24Se2I6Br2O6	Pmm2	Li3XZ	0.09	0.7
Li16S2I6Br2O2	P4mm	Li4XZ2	0.072	0.694
Li32Se8I12Cl14	P-4m2	Li4XZ2	0.074	0.591
Li24Se2I4Br4O6	P4mm	Li3XZ	0.067	0.537
Li16Se1I6Br2O3	P4/mmm	Li4XZ2	0.08	0.596
Li24S2I2Br6O6	Pmm2	Li3XZ	0.055	0.758
Li16S2Br4Cl4O2	P4mm	Li4XZ2	0.099	0.587
Li32Cl8O8F8	Cm	Li4XZ2	0.052	0.6
Li32Br12O8F4	P4mm	Li4XZ2	0.07	0.807
Li32I4O8F12	Cm	Li4XZ2	0.087	0.568
Li24S8I4Br4	Pm-3m	Li3XZ	0.091	0.733
Li24S2I2Br6O6	Cmcm	Li3XZ	0.072	0.588
Li32I12Cl4O8	Cm	Li4XZ2	0.019	0.804
Li16I2Br6O4	P4/nmm	Li4XZ2	0.004	0.722
Li9Cl2O3F1	P4/mmm	Li3XZ	0.056	0.549
Li16Se1I6Br2O3	P4mm	Li4XZ2	0.066	0.59
Li16S1I6Cl2O3	P4mm	Li4XZ2	0.064	0.788

Li32Te2I16O6	Cmcm	Li4XZ2	0.062	0.813
Li14Cl4O4F2	I4/mmm	Li7X2Z3	0.066	0.643
Li24S6I4Cl4O2	Amm2	Li3XZ	0.083	0.83
Li24S2I4Br4O6	Pm	Li3XZ	0.075	0.7
Li16Se3S1I6Br2	P4mm	Li4XZ2	0.097	0.635
Li16S2I6Br2O2	P4mm	Li4XZ2	0.076	0.557
Li9Br2Cl1O3	P4/mmm	Li3XZ	0.011	0.569
Li32I12Cl4O8	P1	Li4XZ2	0.017	0.612
Li24Se6I6Cl2O2	Pma2	Li3XZ	0.098	0.684
Li24S4I4Br4O4	P4mm	Li3XZ	0.079	0.749
Li24S2Br6Cl2O6	Amm2	Li3XZ	0.059	0.671
Li24S8I6Br2	Im-3m	Li3XZ	0.08	0.607
Li24S6I2Br6O2	Pmm2	Li3XZ	0.095	0.718
Li16S2I4Br4O2	P4/mmm	Li4XZ2	0.091	0.828
Li24S6I6Cl2O2	Amm2	Li3XZ	0.082	0.595
Li24S4I6Br2O4	R-3m	Li3XZ	0.082	0.696
Li16Se1I4Br4O3	P4/mmm	Li4XZ2	0.091	0.564
Li14S4I4Cl2	I4mm	Li7X2Z3	0.098	0.65
Li9S3I1Br2	P4/mmm	Li3XZ	0.097	0.61
Li16Te1I6Cl2O3	P4mm	Li4XZ2	0.094	0.501
Li14S2Br4Cl2O2	P4mm	Li7X2Z3	0.096	0.52
Li24S4I4Cl4O4	C2	Li3XZ	0.081	0.554
Li24S2I2Br6O6	Cmme	Li3XZ	0.057	0.762
Li24S2I2Cl6O6	Cmmm	Li3XZ	0.082	0.586
Li14I4O4F2	I4/mmm	Li7X2Z3	0.098	0.812
Li24Se6S2I6Cl2	Pma2	Li3XZ	0.09	0.579
Li24S6Br2Cl6O2	Pmm2	Li3XZ	0.093	0.753
Li16S1I4Br4O3	P4mm	Li4XZ2	0.052	0.723
Li16Se2I6Br2O2	P4mm	Li4XZ2	0.097	0.623
Li32S8I4Cl12	Cm	Li4XZ2	0.059	0.516
Li32Cl12O8F4	P4mm	Li4XZ2	0.045	0.726
Li24S2I4Br4O6	Pmm2	Li3XZ	0.069	0.612
Li16S2I6Br2O2	P4mm	Li4XZ2	0.074	0.632
Li24S4Br8O4	Fm-3m	Li3XZ	0.054	0.603
Li14Br4Cl2O4	P4mm	Li7X2Z3	0.003	0.776
Li16S1I4Br4O3	P4mm	Li4XZ2	0.059	0.739
Li16S1I2Cl6O3	P4mm	Li4XZ2	0.062	0.685
Li16Te1I6Br2O3	P4mm	Li4XZ2	0.085	0.723
Li16Se1I4Br4O3	P4mm	Li4XZ2	0.07	0.895
Li16S1I6Cl2O3	P4mm	Li4XZ2	0.06	0.684
Li14S4I4Cl2	P4/nmm	Li7X2Z3	0.089	0.631
Li16S1Br2Cl6O3	P4mm	Li4XZ2	0.057	0.726
Li32S8I12Br4	Cm	Li4XZ2	0.054	0.683

Li ₂₄ Se ₆ I ₆ Cl ₂ O ₂	Amm2	Li ₃ XZ	0.098	0.551
Li ₁₄ Cl ₄ O ₄ F ₂	P4/nmm	Li ₇ X ₂ Z ₃	0.045	0.772
Li ₂₄ S ₄ I ₈ O ₄	P4/mmm	Li ₃ XZ	0.091	0.697
Li ₁₆ Te ₁ I ₄ Cl ₄ O ₃	P4mm	Li ₄ XZ ₂	0.093	0.566
Li ₁₆ Se ₂ S ₂ I ₆ Br ₂	P4/mmm	Li ₄ XZ ₂	0.09	0.627
Li ₂₄ I ₄ Br ₄ O ₈	P4 ₂ /mmc	Li ₃ XZ	0.056	0.735
Li ₃₂ Se ₈ I ₁₂ Br ₄	P4mm	Li ₄ XZ ₂	0.072	0.56
Li ₂₄ Se ₂ I ₂ Br ₆ O ₆	Cmmm	Li ₃ XZ	0.071	0.684
Li ₂₄ S ₆ Br ₄ Cl ₄ O ₂	Pm	Li ₃ XZ	0.074	0.67
Li ₁₆ Se ₁ Br ₆ Cl ₂ O ₃	P4/mmm	Li ₄ XZ ₂	0.095	0.643
Li ₂₄ S ₂ I ₂ Cl ₆ O ₆	Cmmm	Li ₃ XZ	0.064	0.662
Li ₁₆ S ₁ I ₂ Cl ₆ O ₃	P4mm	Li ₄ XZ ₂	0.061	0.761
Li ₁₆ Te ₁ I ₂ Br ₆ O ₃	P4mm	Li ₄ XZ ₂	0.089	0.61
Li ₁₆ Br ₆ O ₄ F ₂	P4/mmm	Li ₄ XZ ₂	0.077	0.723
Li ₁₆ S ₁ Br ₂ Cl ₆ O ₃	P4mm	Li ₄ XZ ₂	0.059	0.695
Li ₂₄ Se ₂ Br ₆ Cl ₂ O ₆	Cmmm	Li ₃ XZ	0.07	0.693
Li ₁₄ Br ₄ O ₄ F ₂	I4mm	Li ₇ X ₂ Z ₃	0.085	0.854
Li ₁₄ S ₂ I ₄ Br ₂ O ₂	P4mm	Li ₇ X ₂ Z ₃	0.092	0.56
Li ₂₄ S ₄ I ₄ Cl ₄ O ₄	R3m	Li ₃ XZ	0.087	0.731
Li ₂₄ S ₆ I ₄ Cl ₄ O ₂	Pm	Li ₃ XZ	0.08	0.581
Li ₂₄ S ₂ Br ₆ O ₆ F ₂	Pma2	Li ₃ XZ	0.083	0.677
Li ₁₆ I ₄ Cl ₄ O ₄	P4/mmm	Li ₄ XZ ₂	0.028	0.792
Li ₁₆ Se ₁ Br ₄ Cl ₄ O ₃	P4mm	Li ₄ XZ ₂	0.072	0.6
Li ₃₂ Br ₄ Cl ₁₂ O ₈	P4mm	Li ₄ XZ ₂	0	0.664
Li ₃₂ S ₈ I ₁₂ Br ₄	P4mm	Li ₄ XZ ₂	0.074	0.505
Li ₃₂ S ₄ Cl ₁₆ O ₄	Cmmm	Li ₄ XZ ₂	0.077	0.63
Li ₃₂ S ₄ Br ₁₆ O ₄	Amm2	Li ₄ XZ ₂	0.062	0.693
Li ₁₄ S ₂ I ₄ Br ₂ O ₂	P4mm	Li ₇ X ₂ Z ₃	0.083	0.62
Li ₁₄ I ₂ Br ₄ O ₄	P4/nmm	Li ₇ X ₂ Z ₃	0.011	0.6
Li ₂₄ S ₄ I ₄ Br ₄ O ₄	P4mm	Li ₃ XZ	0.095	0.537
Li ₃₂ Cl ₄ O ₈ F ₁₂	P1	Li ₄ XZ ₂	0.076	0.896
Li ₂₄ S ₆ I ₂ Br ₆ O ₂	Cmme	Li ₃ XZ	0.095	0.534
Li ₂₄ Se ₄ Br ₈ O ₄	Fm-3m	Li ₃ XZ	0.078	0.522
Li ₁₆ Se ₄ I ₆ Br ₂	P4/nmm	Li ₄ XZ ₂	0.099	0.656
Li ₁₆ S ₂ I ₄ Br ₄ O ₂	P4mm	Li ₄ XZ ₂	0.078	0.619
Li ₂₄ I ₆ Cl ₂ O ₈	P4/mmm	Li ₃ XZ	0.072	0.648
Li ₃₂ I ₁₂ Br ₄ O ₈	P-4m2	Li ₄ XZ ₂	0.013	0.735
Li ₂₄ S ₆ I ₈ O ₂	P4/mmm	Li ₃ XZ	0.074	0.737
Li ₁₆ Br ₄ Cl ₄ O ₄	P4mm	Li ₄ XZ ₂	0	0.599
Li ₁₆ S ₂ I ₆ Cl ₂ O ₂	P4mm	Li ₄ XZ ₂	0.09	0.884
Li ₁₆ Se ₁ I ₄ Cl ₄ O ₃	P4mm	Li ₄ XZ ₂	0.087	0.591
Li ₃₂ Te ₈ I ₁₂ Br ₄	Cm	Li ₄ XZ ₂	0.081	0.724
Li ₂₄ Se ₆ Br ₄ Cl ₄ O ₂	Ama2	Li ₃ XZ	0.096	0.741

Li ₂₄ Te ₂ I ₄ Br ₄ O ₆	P4mm	Li ₃ XZ	0.086	0.646
Li ₃₂ S ₄ Cl ₁₆ O ₄	P4 ₂ /mmc	Li ₄ XZ ₂	0.076	0.631
Li ₁₄ I ₂ Br ₄ O ₄	I4mm	Li ₇ X ₂ Z ₃	0.013	0.506
Li ₃₂ Br ₁₂ Cl ₄ O ₈	P4mm	Li ₄ XZ ₂	0	0.836
Li ₁₆ Se ₂ I ₆ Br ₂ O ₂	P4mm	Li ₄ XZ ₂	0.098	0.55
Li ₂₄ Se ₄ I ₈ O ₄	Fm-3m	Li ₃ XZ	0.059	0.712
Li ₃₂ S ₆ I ₆ O ₂	P4/mmm	Li ₄ XZ ₂	0.059	0.714
Li ₂₄ Se ₂ S ₆ I ₆ Br ₂	Amm2	Li ₃ XZ	0.091	0.572
Li ₁₆ S ₂ Br ₆ Cl ₂ O ₂	P4mm	Li ₄ XZ ₂	0.091	0.756
Li ₂₄ Se ₄ Br ₆ Cl ₂ O ₄	Ama2	Li ₃ XZ	0.095	0.702
Li ₂₄ S ₆ Br ₆ Cl ₂ O ₂	Cmcm	Li ₃ XZ	0.074	0.554
Li ₂₄ Cl ₆ O ₈ F ₂	P4/mmm	Li ₃ XZ	0.042	0.617
Li ₁₄ Cl ₄ O ₄ F ₂	P4mm	Li ₇ X ₂ Z ₃	0.066	0.779
Li ₂₄ S ₂ Br ₈ O ₆	P4/mmm	Li ₃ XZ	0.047	0.763
Li ₁₆ Te ₁ Br ₄ Cl ₄ O ₃	P4mm	Li ₄ XZ ₂	0.086	0.626
Li ₂₄ S ₄ I ₂ Cl ₆ O ₄	P2	Li ₃ XZ	0.086	0.656
Li ₃₂ S ₈ I ₂ Br ₄	Cm	Li ₄ XZ ₂	0.054	0.581
Li ₂₄ S ₂ I ₂ Br ₆ O ₆	Cmmm	Li ₃ XZ	0.056	0.675
Li ₁₆ Br ₆ O ₄ F ₂	P4/nmm	Li ₄ XZ ₂	0.076	0.524
Li ₁₆ S ₄ I ₆ Cl ₂	P4/nmm	Li ₄ XZ ₂	0.081	0.749
Li ₁₆ S ₃ I ₆ Br ₂ O ₁	P4mm	Li ₄ XZ ₂	0.076	0.543
Li ₃₂ Se ₆ S ₂ I ₁₆	Cmcm	Li ₄ XZ ₂	0.082	0.5
Li ₂₄ I ₂ Br ₆ O ₈	Im-3m	Li ₃ XZ	0.039	0.564
Li ₂₄ Cl ₄ O ₈ F ₄	Fm-3m	Li ₃ XZ	0.091	0.689
Li ₁₄ S ₄ I ₄ Cl ₂	P4/mmm	Li ₇ X ₂ Z ₃	0.098	0.703
Li ₁₆ Br ₄ Cl ₄ O ₄	P4mm	Li ₄ XZ ₂	0	0.591
Li ₂₄ S ₈ I ₆ Br ₂	P4/mmm	Li ₃ XZ	0.08	0.803
Li ₁₆ Se ₁ Br ₄ Cl ₄ O ₃	P4mm	Li ₄ XZ ₂	0.072	0.523
Li ₁₆ Se ₁ S ₃ I ₄ Br ₄	P4mm	Li ₄ XZ ₂	0.095	0.59
Li ₂₄ Cl ₄ O ₈ F ₄	P4/mmm	Li ₃ XZ	0.089	0.704
Li ₂₄ S ₆ I ₆ Br ₂ O ₂	Pma2	Li ₃ XZ	0.078	0.616
Li ₂₄ S ₄ Br ₈ O ₄	Pm-3m	Li ₃ XZ	0.084	0.671
Li ₁₆ Se ₁ I ₆ Cl ₂ O ₃	P4mm	Li ₄ XZ ₂	0.078	0.59
Li ₃₂ S ₈ Cl ₁₂ F ₄	Cm	Li ₄ XZ ₂	0.093	0.595
Li ₂₄ S ₂ I ₂ Cl ₆ O ₆	Pma2	Li ₃ XZ	0.056	0.622
Li ₁₆ I ₂ Br ₆ O ₄	P4mm	Li ₄ XZ ₂	0.007	0.801
Li ₂₄ S ₆ I ₆ Cl ₂ O ₂	Pma2	Li ₃ XZ	0.085	0.76
Li ₁₄ S ₂ Br ₄ Cl ₂ O ₂	P4mm	Li ₇ X ₂ Z ₃	0.096	0.527
Li ₂₄ S ₄ I ₄ Cl ₄ O ₄	P4mm	Li ₃ XZ	0.083	0.819
Li ₁₆ Se ₁ I ₆ Br ₂ O ₃	P4mm	Li ₄ XZ ₂	0.07	0.729
Li ₁₆ S ₂ I ₂ Br ₆ O ₂	P4mm	Li ₄ XZ ₂	0.086	0.603
Li ₂₄ S ₂ Cl ₆ O ₆ F ₂	Pmm2	Li ₃ XZ	0.09	0.641
Li ₂₄ S ₄ I ₂ Br ₆ O ₄	Amm2	Li ₃ XZ	0.08	0.743

Li16S2I2Br6O2	P4mm	Li4XZ2	0.082	0.721
Li24S6I6Cl2O2	Pmm2	Li3XZ	0.088	0.74
Li24Te4Br4Cl4O4	Cm	Li3XZ	0.1	0.608
Li32Se6I16O2	Cmcm	Li4XZ2	0.07	0.607
Li16Se1Br6Cl2O3	P4mm	Li4XZ2	0.066	0.65
Li16S4I4Br4	P4mm	Li4XZ2	0.084	0.514
Li24Br4Cl4O8	P4/mmm	Li3XZ	0.008	0.826
Li24Br6Cl2O8	P4/mmm	Li3XZ	0.013	0.672
Li24Se2Br4Cl4O6	Pmm2	Li3XZ	0.072	0.7
Li16Cl4O4F4	P4mm	Li4XZ2	0.096	0.671
Li16I2Cl6O4	P4/mmm	Li4XZ2	0.011	0.805
Li16Te1Br6Cl2O3	P4mm	Li4XZ2	0.085	0.524
Li32Se6Cl16O2	Cmcm	Li4XZ2	0.096	0.631
Li24S4I6Cl2O4	P2	Li3XZ	0.083	0.566
Li32I12O8F4	Cm	Li4XZ2	0.07	0.815
Li14S4I6	I4/mmm	Li7X2Z3	0.068	0.595
Li14I4Cl2O4	P4mm	Li7X2Z3	0.033	0.58
Li16S2I6Cl2O2	P4mm	Li4XZ2	0.085	0.587
Li16I4Cl4O4	P4mm	Li4XZ2	0.016	0.574
Li32Te2S6I16	Cmcm	Li4XZ2	0.079	0.699
Li32S8I8Br8	P4/mmm	Li4XZ2	0.087	0.722
Li32Cl12O8F4	P4mm	Li4XZ2	0.035	0.57
Li16S2I8O2	P4/nmm	Li4XZ2	0.067	0.651
Li24Se4I6Cl2O4	Pm	Li3XZ	0.087	0.569
Li32Te8Br4Cl12	P1	Li4XZ2	0.086	0.807
Li32S8I12Cl4	P-4m2	Li4XZ2	0.064	0.656
Li16S1Br2Cl6O3	P4mm	Li4XZ2	0.061	0.651
Li16Se3S1I6Br2	P4mm	Li4XZ2	0.096	0.78
Li24S4I2Cl6O4	Amm2	Li3XZ	0.094	0.574
Li16Se3S1I6Br2	P4mm	Li4XZ2	0.097	0.67
Li32S8I12F4	P1	Li4XZ2	0.093	0.614
Li24Se2Br4Cl4O6	Amm2	Li3XZ	0.076	0.641
Li24Se4Br4Cl4O4	Cm	Li3XZ	0.078	0.609
Li24S2Br2Cl6O6	P222_1	Li3XZ	0.054	0.716
Li14S2Br4Cl2O2	P4mm	Li7X2Z3	0.1	0.72
Li16Te1Br2Cl6O3	P4mm	Li4XZ2	0.093	0.678
Li32I12Br4O8	P4mm	Li4XZ2	0.014	0.648
Li16Se2S2I6Br2	P4mm	Li4XZ2	0.089	0.582
Li16Se1I6Br2O3	P4mm	Li4XZ2	0.07	0.613
Li24Se2I4Cl4O6	P4mm	Li3XZ	0.073	0.757
Li16S4I4Cl4	P4/nmm	Li4XZ2	0.099	0.569
Li16I6Br2O4	P4/nmm	Li4XZ2	0.011	0.787
Li16S1I6Br2O3	P4mm	Li4XZ2	0.056	0.652

Li16Se1I4Br4O3	P4mm	Li4XZ2	0.069	0.55
Li16Se1I6Cl2O3	P4mm	Li4XZ2	0.075	0.764
Li24Te2Br2Cl6O6	Pma2	Li3XZ	0.078	0.623
Li16S1I8O3	P4/mmm	Li4XZ2	0.051	0.597
Li32Br4Cl12O8	Cm	Li4XZ2	0	0.577
Li32Se8I8Br8	Cm	Li4XZ2	0.069	0.579
Li16Te1I2Br6O3	P4mm	Li4XZ2	0.085	0.534
Li9S1I2Br1O2	P4/mmm	Li3XZ	0.088	0.845
Li24S2Cl6O6F2	Pma2	Li3XZ	0.083	0.811
Li24Se2I6Cl2O6	Pmm2	Li3XZ	0.09	0.659
Li24Te4S4I6Cl2	C2/c	Li3XZ	0.1	0.634
Li24Te2I2Cl6O6	Pmm2	Li3XZ	0.092	0.652
Li24Se2Br6Cl2O6	Pma2	Li3XZ	0.074	0.601
Li14S2I6O2	P4/mmm	Li7X2Z3	0.083	0.654
Li16S1I2Cl6O3	P4mm	Li4XZ2	0.065	0.603
Li16S2Br8O2	P4/mmm	Li4XZ2	0.085	0.535
Li9S3I2Br1	P4/mmm	Li3XZ	0.082	0.555
Li16Te1I6Cl2O3	P4mm	Li4XZ2	0.086	0.636
Li16S3I6Cl2O1	P4mm	Li4XZ2	0.083	0.875
Li24Se2I6Br2O6	Cmmm	Li3XZ	0.078	0.687
Li24S2I4Cl4O6	Pm	Li3XZ	0.076	0.758
Li24S4I8O4	P4/mmm	Li3XZ	0.075	0.545
Li16Br2Cl6O4	P4/mmm	Li4XZ2	0	0.609
Li24Te2I4Br4O6	Cmm2	Li3XZ	0.089	0.734
Li14Se2S2I6	P4/mmm	Li7X2Z3	0.086	0.739
Li9Se1S2I2Br1	P4mm	Li3XZ	0.099	0.618
Li9S1Br1Cl2O2	P4mm	Li3XZ	0.093	0.767
Li16S3I4Br4O1	P4mm	Li4XZ2	0.088	0.754
Li16Se1Br4Cl4O3	P4mm	Li4XZ2	0.075	0.74
Li32Te8I12Br4	Cm	Li4XZ2	0.091	0.638
Li16I4Br4O4	I4mm	Li4XZ2	0.01	0.737
Li24S2I4Cl4O6	Amm2	Li3XZ	0.076	0.758
Li24S4Br6Cl2O4	Cmm2	Li3XZ	0.083	0.578
Li16Se1S3I6Br2	P4mm	Li4XZ2	0.083	0.81
Li24Te2I4Cl4O6	Cmm2	Li3XZ	0.095	0.527
Li14S4I2Br4	P4mm	Li7X2Z3	0.094	0.645
Li32I12Br4O8	Cm	Li4XZ2	0.013	0.561
Li24S2Br2Cl6O6	Cmmm	Li3XZ	0.071	0.6
Li32I8Cl8O8	Pmm2	Li4XZ2	0.02	0.658
Li24S2I2Cl6O6	Pma2	Li3XZ	0.072	0.69
Li24Te4S4Br4Cl4	C2	Li3XZ	0.099	0.603
Li24S2I6Br2O6	Pmm2	Li3XZ	0.067	0.563
Li24Te2S6I4Cl4	Pm	Li3XZ	0.096	0.73

Li ₂₄ Br ₂ Cl ₆ O ₈	Im-3m	Li ₃ XZ	0.003	0.822
Li ₂₄ Te ₂ Br ₄ Cl ₄ O ₆	Cmm2	Li ₃ XZ	0.085	0.537
Li ₃₂ I ₄ Cl ₁₂ O ₈	P4mm	Li ₄ XZ ₂	0.015	0.577
Li ₂₄ S ₂ Cl ₈ O ₆	P4/mmm	Li ₃ XZ	0.072	0.762
Li ₁₆ S ₁ Br ₂ Cl ₆ O ₃	P4mm	Li ₄ XZ ₂	0.058	0.71
Li ₁₆ S ₂ Br ₄ Cl ₄ O ₂	P4mm	Li ₄ XZ ₂	0.096	0.565
Li ₂₄ S ₂ I ₄ Br ₄ O ₆	Ama2	Li ₃ XZ	0.073	0.816
Li ₉ S ₂ I ₁ Br ₂ O ₁	P4/mmm	Li ₃ XZ	0.097	0.784
Li ₃₂ Te ₂ Br ₁₆ O ₆	Cmcm	Li ₄ XZ ₂	0.072	0.725
Li ₁₆ I ₆ Br ₂ O ₄	P4/nmm	Li ₄ XZ ₂	0.014	0.619
Li ₉ Se ₁ S ₂ I ₂ Br ₁	P4/mmm	Li ₃ XZ	0.097	0.715
Li ₁₄ I ₂ Br ₄ O ₄	P4mm	Li ₇ X ₂ Z ₃	0.027	0.571
Li ₂₄ S ₄ I ₄ Br ₄ O ₄	R3m	Li ₃ XZ	0.078	0.563
Li ₂₄ Br ₂ Cl ₆ O ₈	P4/mmm	Li ₃ XZ	0.003	0.501
Li ₂₄ S ₆ I ₄ Br ₄ O ₂	Pm	Li ₃ XZ	0.072	0.676
Li ₁₆ Se ₁ I ₂ Cl ₆ O ₃	P4mm	Li ₄ XZ ₂	0.074	0.633
Li ₁₆ S ₂ I ₆ Cl ₂ O ₂	P4mm	Li ₄ XZ ₂	0.085	0.722
Li ₁₄ Cl ₄ O ₄ F ₂	I4mm	Li ₇ X ₂ Z ₃	0.067	0.583
Li ₃₂ I ₁₂ Br ₄ O ₈	Pmm2	Li ₄ XZ ₂	0.013	0.754
Li ₂₄ Se ₄ I ₄ Br ₄ O ₄	Cm	Li ₃ XZ	0.078	0.671
Li ₁₆ Te ₁ I ₄ Br ₄ O ₃	P4mm	Li ₄ XZ ₂	0.083	0.774
Li ₂₄ Te ₂ S ₆ I ₄ Cl ₄	Ama2	Li ₃ XZ	0.097	0.643
Li ₁₄ I ₄ Br ₂ O ₄	P4mm	Li ₇ X ₂ Z ₃	0.03	0.77
Li ₂₄ Se ₆ I ₆ Cl ₂ O ₂	Cmme	Li ₃ XZ	0.093	0.687
Li ₁₆ Te ₁ I ₆ Br ₂ O ₃	P4mm	Li ₄ XZ ₂	0.086	0.608
Li ₁₆ Te ₁ Br ₂ Cl ₆ O ₃	P4mm	Li ₄ XZ ₂	0.096	0.773
Li ₂₄ I ₄ Br ₄ O ₈	P4/mmm	Li ₃ XZ	0.057	0.845
Li ₂₄ S ₄ I ₄ Br ₄ O ₄	P4mm	Li ₃ XZ	0.094	0.709
Li ₁₄ Cl ₄ O ₄ F ₂	P4mm	Li ₇ X ₂ Z ₃	0.068	0.684
Li ₃₂ Br ₁₂ O ₈ F ₄	Cm	Li ₄ XZ ₂	0.049	0.792
Li ₁₆ S ₂ Br ₆ Cl ₂ O ₂	P4mm	Li ₄ XZ ₂	0.091	0.636
Li ₂₄ S ₂ I ₆ Cl ₂ O ₆	P222_1	Li ₃ XZ	0.075	0.791
Li ₂₄ S ₄ Br ₆ Cl ₂ O ₄	C2/c	Li ₃ XZ	0.069	0.663
Li ₂₄ Se ₂ I ₆ Cl ₂ O ₆	Pma2	Li ₃ XZ	0.077	0.836
Li ₂₄ S ₄ I ₄ Br ₄ O ₄	Cm	Li ₃ XZ	0.069	0.767
Li ₂₄ Se ₆ S ₂ I ₈	P4/mmm	Li ₃ XZ	0.094	0.556
Li ₁₆ S ₃ I ₂ Br ₆ O ₁	P4mm	Li ₄ XZ ₂	0.091	0.518
Li ₁₆ Te ₁ Br ₆ Cl ₂ O ₃	P4mm	Li ₄ XZ ₂	0.085	0.506
Li ₂₄ S ₆ Br ₆ Cl ₂ O ₂	Cmme	Li ₃ XZ	0.072	0.677
Li ₁₆ Se ₁ S ₃ I ₄ Br ₄	P4mm	Li ₄ XZ ₂	0.092	0.676
Li ₂₄ Se ₂ I ₆ Cl ₂ O ₆	Cmme	Li ₃ XZ	0.086	0.713
Li ₂₄ Se ₂ I ₂ Cl ₆ O ₆	Cmme	Li ₃ XZ	0.087	0.604
Li ₁₆ Cl ₄ O ₄ F ₄	P4/nmm	Li ₄ XZ ₂	0.077	0.711

Li32Se4Cl16O4	Amm2	Li4XZ2	0.086	0.608
Li24S4I6Cl2O4	C2/c	Li3XZ	0.087	0.626
Li24I4Cl4O8	P4/mmm	Li3XZ	0.055	0.707
Li24S2I4Cl4O6	P4mm	Li3XZ	0.061	0.732
Li16S2I2Br6O2	P4mm	Li4XZ2	0.081	0.788
Li16Se1I6Cl2O3	P4mm	Li4XZ2	0.07	0.69
Li14S2I2Br4O2	P4mm	Li7X2Z3	0.087	0.583
Li24Se2I8O6	Im-3m	Li3XZ	0.092	0.81
Li24Se2I2Br6O6	Pmm2	Li3XZ	0.078	0.725
Li16S3I4Br4O1	P4mm	Li4XZ2	0.089	0.544
Li16Se2I6Br2O2	P4mm	Li4XZ2	0.097	0.724
Li24S2Br8O6	P4/mmm	Li3XZ	0.063	0.726
Li16S1I6Br2O3	P4mm	Li4XZ2	0.052	0.598
Li14S2I4Br2O2	P4mm	Li7X2Z3	0.096	0.734
Li24S2I4Cl4O6	Pm	Li3XZ	0.075	0.624
Li14S4I4Br2	P4/nmm	Li7X2Z3	0.077	0.68
Li16S2I2Br6O2	P4mm	Li4XZ2	0.081	0.652
Li24S2Br4Cl4O6	P4mm	Li3XZ	0.051	0.794
Li32I12O8F4	P4mm	Li4XZ2	0.079	0.727
Li24Cl6O8F2	Im-3m	Li3XZ	0.045	0.714
Li32Te2S6I16	P4/mmm	Li4XZ2	0.091	0.721
Li16S1Br4Cl4O3	P4mm	Li4XZ2	0.056	0.61
Li16S3I6Cl2O1	P4mm	Li4XZ2	0.089	0.735
Li24S2Br6Cl2O6	Cmme	Li3XZ	0.05	0.601
Li16S3I4Br4O1	P4mm	Li4XZ2	0.088	0.715
Li24Se4I4Cl4O4	P4mm	Li3XZ	0.1	0.755
Li32Te8Cl12F4	Cm	Li4XZ2	0.096	0.583
Li16S1Br6Cl2O3	P4/mmm	Li4XZ2	0.064	0.554
Li32Te4S4I16	Amm2	Li4XZ2	0.093	0.819
Li16S3I2Br6O1	P4mm	Li4XZ2	0.095	0.581
Li24S6I6Br2O2	Cmme	Li3XZ	0.082	0.815
Li24Te2S6I6Cl2	Cmme	Li3XZ	0.087	0.761
Li32I4Cl12O8	P-4m2	Li4XZ2	0.018	0.703
Li24Se2I6Br2O6	Pma2	Li3XZ	0.074	0.524
Li24S2Br2Cl6O6	Cmme	Li3XZ	0.054	0.686
Li32I4Cl12O8	P4mm	Li4XZ2	0.015	0.775
Li14Br4Cl2O4	I4mm	Li7X2Z3	0.007	0.662
Li32S4Cl16O4	Amm2	Li4XZ2	0.07	0.529
Li24Se6I4Cl4O2	Pm	Li3XZ	0.095	0.665
Li16S4I4Br4	P4/mmm	Li4XZ2	0.081	0.591
Li16S1I6Cl2O3	P4/mmm	Li4XZ2	0.072	0.546
Li24Se2Cl6O6F2	Amm2	Li3XZ	0.09	0.582
Li16Br6O4F2	P4/mmm	Li4XZ2	0.077	0.856

Li16S2I6Br2O2	P4/mmm	Li4XZ2	0.079	0.569
Li16Te1I2Br6O3	P4mm	Li4XZ2	0.091	0.703
Li24I4Br4O8	Fm-3m	Li3XZ	0.059	0.569
Li16Se2S2I6Br2	P4mm	Li4XZ2	0.092	0.715
Li14Br2Cl4O4	P4/nmm	Li7X2Z3	0	0.754
Li16Se1S3I4Br4	P4mm	Li4XZ2	0.093	0.64
Li16Te1I4Br4O3	P4mm	Li4XZ2	0.081	0.713
Li16Br4Cl4O4	I4mm	Li4XZ2	0	0.786
Li16Br4Cl4O4	P4mm	Li4XZ2	0	0.768
Li24Se2Cl8O6	Im-3m	Li3XZ	0.091	0.737
Li16Se1Br6Cl2O3	P4mm	Li4XZ2	0.07	0.735
Li24Se2Cl6O6F2	Pma2	Li3XZ	0.098	0.566
Li24Br4Cl4O8	P4/mmm	Li3XZ	0.009	0.661
Li16Te1I4Cl4O3	P4mm	Li4XZ2	0.097	0.758
Li32Se8I4Cl12	Cm	Li4XZ2	0.077	0.777
Li24S2I4Br4O6	Cmm2	Li3XZ	0.061	0.574
Li16Se1S3I4Br4	P4mm	Li4XZ2	0.092	0.719
Li24Se2Br2Cl6O6	Pma2	Li3XZ	0.075	0.844
Li16S1I4Br4O3	P4mm	Li4XZ2	0.059	0.602
Li16S4I6Cl2	P4/nmm	Li4XZ2	0.089	0.572
Li32Se6Br16O2	Cmcm	Li4XZ2	0.088	0.73
Li24S2Br6O6F2	Pmm2	Li3XZ	0.085	0.613
Li24S8I6Cl2	Im-3m	Li3XZ	0.095	0.776
Li16Te1I4Br4O3	P4mm	Li4XZ2	0.091	0.51
Li16Br6Cl2O4	P4/nmm	Li4XZ2	0	0.675
Li16Cl4O4F4	P4mm	Li4XZ2	0.096	0.666
Li16Te1I6Cl2O3	P4mm	Li4XZ2	0.094	0.781
Li9S1Br2Cl1O2	P4mm	Li3XZ	0.091	0.643
Li16Se1S3I6Cl2	P4mm	Li4XZ2	0.097	0.736
Li24Se4I4Br4O4	R3m	Li3XZ	0.092	0.663
Li32Br16O8	I4/mmm	Li4XZ2	0	0.672
Li24Se6I6Br2O2	Amm2	Li3XZ	0.099	0.687
Li24Se2I2Br6O6	Cmmm	Li3XZ	0.097	0.565
Li24Se2Cl6O6F2	Cmcm	Li3XZ	0.094	0.564
Li24Se4Br4Cl4O4	C2	Li3XZ	0.086	0.539
Li32S2Cl16O6	P4/mmm	Li4XZ2	0.045	0.585
Li24Se2Br2Cl6O6	P222_1	Li3XZ	0.078	0.737
Li24S2Cl4O6F4	Pm	Li3XZ	0.088	0.754
Li16S1Br6Cl2O3	P4mm	Li4XZ2	0.055	0.551
Li24I4Br4O8	Pm-3m	Li3XZ	0.056	0.667
Li16Se1I4Cl4O3	P4mm	Li4XZ2	0.089	0.622
Li16Se1I6Br2O3	P4mm	Li4XZ2	0.067	0.59
Li16Se2S2I6Br2	P4mm	Li4XZ2	0.091	0.637

Li16S11I6Br2O3	P4/mmm	Li4XZ2	0.056	0.733
Li24S6I2Br6O2	Amm2	Li3XZ	0.1	0.53
Li24Se2I2Br6O6	Cmme	Li3XZ	0.073	0.725
Li24S2Br6Cl2O6	Cmmm	Li3XZ	0.066	0.67
Li24Br6Cl2O8	P4/mmm	Li3XZ	0.013	0.7
Li24Se6S2I8	Im-3m	Li3XZ	0.094	0.573
Li16Te1I6Cl2O3	P4mm	Li4XZ2	0.086	0.55
Li16S2I2Br6O2	P4/mmm	Li4XZ2	0.088	0.735
Li32Cl12O8F4	P4mm	Li4XZ2	0.054	0.582
Li24S6I4Br4O2	Pm	Li3XZ	0.078	0.797
Li16Te1I2Br6O3	P4mm	Li4XZ2	0.084	0.784
Li14Br2Cl4O4	I4/mmm	Li7X2Z3	0.004	0.524
Li24Se2S6I6Br2	Pma2	Li3XZ	0.091	0.768
Li9S1Br3O2	P4/mmm	Li3XZ	0.084	0.59
Li24S4I4Br4O4	Pmma	Li3XZ	0.096	0.661
Li32I4Br12O8	P4mm	Li4XZ2	0.005	0.683
Li24S6Br2Cl6O2	Cmcm	Li3XZ	0.083	0.797
Li24S6I4Br4O2	Pmm2	Li3XZ	0.087	0.847
Li32Se8I8Cl8	Cm	Li4XZ2	0.069	0.793
Li24S4I4Br4O4	P4mm	Li3XZ	0.079	0.726
Li16Te1I6Cl2O3	P4mm	Li4XZ2	0.092	0.655
Li24Se2Br6O6F2	Amm2	Li3XZ	0.092	0.862
Li14S2I2Br4O2	P4mm	Li7X2Z3	0.085	0.616
Li24Se2Br2Cl6O6	Cmmm	Li3XZ	0.078	0.828
Li24Se4Br4Cl4O4	C2	Li3XZ	0.086	0.799
Li16Se1Br2Cl6O3	P4mm	Li4XZ2	0.073	0.805
Li24Se6I2Br6O2	Cmme	Li3XZ	0.096	0.777
Li24S2Cl6O6F2	Pma2	Li3XZ	0.081	0.592
Li24Se2Br2Cl6O6	Cmcm	Li3XZ	0.07	0.632
Li16Se2I6Br2O2	P4mm	Li4XZ2	0.093	0.573
Li24S4I6Cl2O4	Ama2	Li3XZ	0.083	0.599
Li16Te1I6Br2O3	P4mm	Li4XZ2	0.088	0.686
Li16Se1Br4Cl4O3	P4mm	Li4XZ2	0.069	0.557
Li24S6I6Cl2O2	Cmmm	Li3XZ	0.087	0.67
Li24Se2I2Cl6O6	P222_1	Li3XZ	0.086	0.829
Li32I8Cl8O8	Cm	Li4XZ2	0.023	0.777
Li32S2I16O6	Cmcm	Li4XZ2	0.031	0.84
Li24S6I6Cl2O2	Cmmm	Li3XZ	0.092	0.627
Li24I4Cl4O8	P4_2/mmc	Li3XZ	0.053	0.696
Li24S4I4Cl4O4	Cm	Li3XZ	0.076	0.757
Li16Se1S3I6Cl2	P4/mmm	Li4XZ2	0.097	0.606
Li24Se4S4I8	P4_2/mmc	Li3XZ	0.086	0.573
Li16S2I4Br4O2	P4mm	Li4XZ2	0.077	0.679

Li32Br4O8F12	P1	Li4XZ2	0.077	0.727
Li16S3I6Cl2O1	P4/mmm	Li4XZ2	0.094	0.723
Li32S4I16O4	Cmmm	Li4XZ2	0.04	0.733
Li16S1I6Br2O3	P4mm	Li4XZ2	0.055	0.71
Li16S2I4Cl4O2	P4mm	Li4XZ2	0.096	0.626
Li16Se1S3I6Br2	P4mm	Li4XZ2	0.081	0.842
Li16Se1S3I6Br2	P4/mmm	Li4XZ2	0.083	0.555
Li14S4I2Br4	P4/mmm	Li7X2Z3	0.099	0.505
Li16Br6Cl2O4	P4/nmm	Li4XZ2	0	0.79
Li24S4I2Br6O4	Ama2	Li3XZ	0.085	0.57
Li24S6Br4Cl4O2	Pmma	Li3XZ	0.095	0.623
Li32I4Cl12O8	Cm	Li4XZ2	0.012	0.692
Li16I4Cl4O4	P4mm	Li4XZ2	0.016	0.687
Li16Te1I4Cl4O3	P4mm	Li4XZ2	0.095	0.572
Li16S2I2Br6O2	P4mm	Li4XZ2	0.084	0.682
Li24Se2Br8O6	P4/mmm	Li3XZ	0.092	0.788
Li16S3I2Br6O1	P4mm	Li4XZ2	0.095	0.829
Li16S2I4Br4O2	P4mm	Li4XZ2	0.081	0.561
Li24S2I4Cl4O6	Pmm2	Li3XZ	0.07	0.513
Li24Se4I2Cl6O4	Pm	Li3XZ	0.093	0.82
Li24S2I2Cl6O6	Cmcm	Li3XZ	0.069	0.638
Li24S4Br4Cl4O4	P4mm	Li3XZ	0.084	0.508
Li16Br4Cl4O4	P4/nmm	Li4XZ2	0	0.767
Li16Br6Cl2O4	P4mm	Li4XZ2	0	0.579
Li24S6I4Cl4O2	Ama2	Li3XZ	0.082	0.659
Li16S2I6Br2O2	P4/mmm	Li4XZ2	0.079	0.75
Li32Te4S4I16	P4_2/mmc	Li4XZ2	0.089	0.651
Li24I8O8	Pm-3m	Li3XZ	0.087	0.634
Li16Se1S3I4Br4	P4mm	Li4XZ2	0.093	0.509
Li16S4I4Br4	P4mm	Li4XZ2	0.086	0.519
Li32Se8I12Cl4	Cm	Li4XZ2	0.069	0.597
Li32S4Br16O4	P4/mmm	Li4XZ2	0.085	0.752
Li32Se6S2I16	P4/mmm	Li4XZ2	0.082	0.592
Li16S2Br6Cl2O2	P4mm	Li4XZ2	0.092	0.752
Li24Se2Br2Cl6O6	Pmm2	Li3XZ	0.072	0.558
Li32I4Br12O8	Pmm2	Li4XZ2	0.007	0.796
Li32I12Br4O8	P4mm	Li4XZ2	0.013	0.536
Li16S1I2Cl6O3	P4mm	Li4XZ2	0.064	0.511
Li16Se1Br6Cl2O3	P4mm	Li4XZ2	0.069	0.769
Li24S4I2Br6O4	P4/nmm	Li3XZ	0.087	0.627
Li24Se2S6I6Br2	Cmcm	Li3XZ	0.091	0.857
Li24Se2I4Br4O6	Pmm2	Li3XZ	0.08	0.679
Li16S3I2Br6O1	P4mm	Li4XZ2	0.091	0.509

Li14Br2Cl4O4	P4mm	Li7X2Z3	0.001	0.828
Li16S4I4Cl4	P4/mmm	Li4XZ2	0.099	0.813
Li24S2Cl6O6F2	Amm2	Li3XZ	0.076	0.589
Li24Te2Br6Cl2O6	Pmm2	Li3XZ	0.085	0.782
Li16S1Br2Cl6O3	P4mm	Li4XZ2	0.059	0.552
Li16S4I6Br2	P4/nmm	Li4XZ2	0.074	0.695
Li24Se2I2Br6O6	Pmm2	Li3XZ	0.067	0.748
Li14Se2S2I4Br2	P4/mmm	Li7X2Z3	0.099	0.674
Li24Se2I2Cl6O6	Cmmm	Li3XZ	0.084	0.791
Li16Te1Br4Cl4O3	P4mm	Li4XZ2	0.091	0.752
Li24S2I8O6	Im-3m	Li3XZ	0.08	0.585
Li24S4Br4Cl4O4	P4mm	Li3XZ	0.084	0.841
Li16Se1I6Br2O3	P4/mmm	Li4XZ2	0.086	0.593
Li24S4Br2Cl6O4	Amm2	Li3XZ	0.092	0.622
Li16S3I6Br2O1	P4mm	Li4XZ2	0.077	0.886
Li16S3I6Br2O1	P4/mmm	Li4XZ2	0.083	0.829
Li24Cl8O8	Pm-3m	Li3XZ	0	0.667
Li24Se6Br4Cl4O2	Amm2	Li3XZ	0.094	0.74
Li16S1I2Br6O3	P4mm	Li4XZ2	0.053	0.85
Li16Br4Cl4O4	P4mm	Li4XZ2	0	0.502
Li24S4I2Br6O4	P4mm	Li3XZ	0.096	0.751
Li16S1I6Br2O3	P4mm	Li4XZ2	0.056	0.603
Li24Se6S2I8	P4/mmm	Li3XZ	0.094	0.696
Li16Se1I4Cl4O3	P4mm	Li4XZ2	0.085	0.62
Li32I8Br8O8	P4/mmm	Li4XZ2	0.014	0.604
Li24Se4I2Br6O4	Ama2	Li3XZ	0.092	0.642
Li32I12O8F4	P-4m2	Li4XZ2	0.085	0.535
Li24S4I2Cl6O4	Pm	Li3XZ	0.078	0.771
Li24I6Br2O8	P4/mmm	Li3XZ	0.073	0.53
Li14I2Cl4O4	I4mm	Li7X2Z3	0.01	0.611
Li24I2Cl6O8	P4/mmm	Li3XZ	0.026	0.589
Li24Br2Cl6O8	P4/mmm	Li3XZ	0.002	0.744
Li16S1I4Br4O3	P4mm	Li4XZ2	0.058	0.608
Li32I12Cl4O8	P4mm	Li4XZ2	0.02	0.717
Li16Se1Br2Cl6O3	P4mm	Li4XZ2	0.071	0.563
Li16I4Br4O4	P4/mmm	Li4XZ2	0.008	0.669
Li16S2I4Cl4O2	P4mm	Li4XZ2	0.095	0.588
Li24Te2I2Cl6O6	Pma2	Li3XZ	0.079	0.625
Li16I4Br4O4	P4mm	Li4XZ2	0.011	0.55
Li24S4Br4Cl4O4	Pmm2	Li3XZ	0.071	0.537
Li32S4I16O4	P4_2/mmc	Li4XZ2	0.05	0.577
Li16Te1I4Cl4O3	P4mm	Li4XZ2	0.087	0.683
Li14I4Cl2O4	I4mm	Li7X2Z3	0.051	0.587

Li24Br4Cl4O8	P4/mmm	Li3XZ	0.007	0.687
Li24S6I2Br6O2	Pma2	Li3XZ	0.082	0.552
Li24Se2Br2Cl6O6	Pmm2	Li3XZ	0.077	0.698
Li24Se4Br6Cl2O4	Pm	Li3XZ	0.087	0.502
Li16I6Cl2O4	P4mm	Li4XZ2	0.021	0.682
Li24S4I4Cl4O4	R3m	Li3XZ	0.087	0.853
Li24Se4S4I8	Fm-3m	Li3XZ	0.084	0.756
Li32Se4Br16O4	Amm2	Li4XZ2	0.078	0.743
Li32Br12Cl4O8	Pmm2	Li4XZ2	0	0.641
Li24Te4Se4I4Br4	Pmm2	Li3XZ	0.099	0.554
Li24Se6I2Br6O2	Pma2	Li3XZ	0.099	0.726
Li14S4I2Br4	P4mm	Li7X2Z3	0.093	0.61
Li16Se1S3I6Br2	P4mm	Li4XZ2	0.083	0.596
Li24S4I6Cl2O4	Cmm2	Li3XZ	0.084	0.571
Li24S2Cl6O6F2	Cmme	Li3XZ	0.092	0.706
Li32Se2Cl16O6	Cmcm	Li4XZ2	0.055	0.514
Li24S2I2Cl6O6	Cmme	Li3XZ	0.068	0.555
Li16Br6Cl2O4	P4mm	Li4XZ2	0	0.544
Li16Se2S2I6Br2	P4mm	Li4XZ2	0.09	0.747
Li16I6Cl2O4	P4/nmm	Li4XZ2	0.011	0.719
Li24Te2S6I2Br6	Pmm2	Li3XZ	0.098	0.786
Li16Cl4O4F4	P4/mmm	Li4XZ2	0.078	0.7
Li16Se1Br2Cl6O3	P4mm	Li4XZ2	0.075	0.753
Li16S2Br8O2	P4/nmm	Li4XZ2	0.084	0.773
Li24S2I2Br6O6	P222_1	Li3XZ	0.057	0.889
Li24S6I2Cl6O2	Pmm2	Li3XZ	0.094	0.686
Li24Br4Cl4O8	Fm-3m	Li3XZ	0.009	0.621
Li24Br8O8	Pm-3m	Li3XZ	0.017	0.797
Li24S6I6Br2O2	Cmmm	Li3XZ	0.087	0.554
Li32Se8I12Cl4	Cm	Li4XZ2	0.067	0.695
Li14I2Cl4O4	I4/mmm	Li7X2Z3	0.04	0.502
Li24Se2I4Cl4O6	Pm	Li3XZ	0.084	0.726
Li16Se1S3I6Cl2	P4/mmm	Li4XZ2	0.098	0.694
Li16Se1Br6Cl2O3	P4mm	Li4XZ2	0.071	0.655
Li16I4Br4O4	P4/nmm	Li4XZ2	0.008	0.642
Li24S4Br4Cl4O4	R3m	Li3XZ	0.086	0.512
Li16S2I6Cl2O2	P4/mmm	Li4XZ2	0.096	0.722
Li16Se2S2I6Br2	P4/mmm	Li4XZ2	0.09	0.673
Li16Se1I2Cl6O3	P4mm	Li4XZ2	0.074	0.504
Li24S8I4Br4	P4/mmm	Li3XZ	0.091	0.756
Li24S2I8O6	P4/mmm	Li3XZ	0.074	0.58
Li24S2I4Br4O6	P4_2/mcm	Li3XZ	0.08	0.617
Li24Se4Br4Cl4O4	Pmm2	Li3XZ	0.098	0.75

Li16Se1Br2Cl6O3	P4mm	Li4XZ2	0.072	0.813
Li16S3I6Cl2O1	P4mm	Li4XZ2	0.093	0.838
Li16Se1I4Cl4O3	P4mm	Li4XZ2	0.09	0.706
Li16I4Br4O4	P4mm	Li4XZ2	0.01	0.773
Li16Se1I2Cl6O3	P4mm	Li4XZ2	0.089	0.769
Li24I2Cl6O8	Im-3m	Li3XZ	0.031	0.642
Li16Se2S2I6Br2	P4mm	Li4XZ2	0.09	0.82
Li16Te1I4Br4O3	P4mm	Li4XZ2	0.081	0.609
Li14S4I4Br2	P4/mmm	Li7X2Z3	0.081	0.828
Li16I6Cl2O4	P4/mmm	Li4XZ2	0.024	0.842
Li16S1Br6Cl2O3	P4mm	Li4XZ2	0.054	0.649
Li16Se1S3I6Cl2	P4mm	Li4XZ2	0.097	0.662
Li16Te1Br4Cl4O3	P4mm	Li4XZ2	0.088	0.579
Li32Br12O8F4	P4mm	Li4XZ2	0.056	0.649
Li24S4I6Br2O4	Amm2	Li3XZ	0.078	0.641
Li16Br4Cl4O4	P4mm	Li4XZ2	0	0.565
Li16Se1I4Cl4O3	P4mm	Li4XZ2	0.081	0.705
Li24Se2I2Cl6O6	Amm2	Li3XZ	0.083	0.693
Li16Cl6O4F2	P4mm	Li4XZ2	0.054	0.577
Li14S2Br6O2	P4/nmm	Li7X2Z3	0.089	0.82
Li16Se1Br2Cl6O3	P4mm	Li4XZ2	0.07	0.584
Li24S6I6Br2O2	Pma2	Li3XZ	0.081	0.549
Li24S6I6Cl2O2	Pmm2	Li3XZ	0.087	0.554
Li14Br4Cl2O4	P4/mmm	Li7X2Z3	0.008	0.545
Li16I6Cl2O4	P4/nmm	Li4XZ2	0.023	0.693
Li24Se2Cl6O6F2	Pma2	Li3XZ	0.099	0.71
Li16Se2I8O2	P4/mmm	Li4XZ2	0.096	0.503
Li16Se1S3I6Br2	P4mm	Li4XZ2	0.083	0.73
Li24S4I4Br4O4	C2	Li3XZ	0.08	0.764
Li14S2I2Br4O2	P4mm	Li7X2Z3	0.1	0.879
Li16Se1I2Br6O3	P4mm	Li4XZ2	0.067	0.718
Li24I6Br2O8	P4/mmm	Li3XZ	0.073	0.704
Li24S6I2Br6O2	Cmcm	Li3XZ	0.073	0.604
Li16S1I6Cl2O3	P4mm	Li4XZ2	0.063	0.731
Li16Se2I6Cl2O2	P4mm	Li4XZ2	0.099	0.548
Li16S1I2Br6O3	P4mm	Li4XZ2	0.054	0.586
Li14I4Cl2O4	P4mm	Li7X2Z3	0.033	0.813
Li24Cl4O8F4	P4/mmm	Li3XZ	0.09	0.546
Li14S2I4Cl2O2	P4mm	Li7X2Z3	0.097	0.838
Li16S3I6Br2O1	P4/mmm	Li4XZ2	0.08	0.525
Li16S1Br4Cl4O3	P4mm	Li4XZ2	0.059	0.812
Li16Se1S3I6Cl2	P4mm	Li4XZ2	0.097	0.835
Li16S1I4Cl4O3	P4mm	Li4XZ2	0.073	0.662

Li16S2I6Br2O2	P4mm	Li4XZ2	0.074	0.709
Li16S1I2Br6O3	P4/mmm	Li4XZ2	0.061	0.72
Li14I2Br4O4	I4/mmm	Li7X2Z3	0.039	0.629
Li24I4Cl4O8	Pm-3m	Li3XZ	0.051	0.577
Li16Se1I8O3	P4/mmm	Li4XZ2	0.074	0.63
Li24Se2S6I8	Im-3m	Li3XZ	0.077	0.683
Li16Br6O4F2	P4mm	Li4XZ2	0.07	0.751
Li32S2Br16O6	P4/mmm	Li4XZ2	0.035	0.549
Li24Se2I4Cl4O6	Pm	Li3XZ	0.084	0.597
Li16Se1S3I6Cl2	P4mm	Li4XZ2	0.098	0.521
Li32S8I12Cl4	P4mm	Li4XZ2	0.081	0.621
Li16Se3S1I6Br2	P4mm	Li4XZ2	0.096	0.706
Li16S2I4Br4O2	P4mm	Li4XZ2	0.076	0.557
Li16S3I2Br6O1	P4/mmm	Li4XZ2	0.093	0.595
Li24S2I4Cl4O6	Cmmm	Li3XZ	0.091	0.737
Li16Se1Br6Cl2O3	P4mm	Li4XZ2	0.067	0.644
Li24S4Br2Cl6O4	Cmm2	Li3XZ	0.088	0.757
Li16Br6Cl2O4	P4/mmm	Li4XZ2	0	0.636
Li32S8Br12Cl4	P-4m2	Li4XZ2	0.075	0.695
Li32S8I12F4	Cm	Li4XZ2	0.098	0.871
Li24S4I6Br2O4	P4mm	Li3XZ	0.093	0.605
Li16S1I2Br6O3	P4mm	Li4XZ2	0.052	0.528
Li24S4I4Br4O4	P4mm	Li3XZ	0.095	0.572
Li16Se1I2Br6O3	P4mm	Li4XZ2	0.065	0.678
Li24Se6I6Br2O2	Pmm2	Li3XZ	0.096	0.744
Li24S6I4Br4O2	Pmma	Li3XZ	0.082	0.785
Li24Se2I6Br2O6	Amm2	Li3XZ	0.089	0.678
Li32S8Br12F4	Cm	Li4XZ2	0.093	0.736
Li32S8I4Br12	P4mm	Li4XZ2	0.075	0.607
Li14Br2Cl4O4	I4mm	Li7X2Z3	0	0.742
Li16S1Br4Cl4O3	P4mm	Li4XZ2	0.058	0.5
Li24S2I2Cl6O6	P222_1	Li3XZ	0.067	0.62
Li24Te2I2Br6O6	Pmm2	Li3XZ	0.085	0.808
Li16I4Cl4O4	P4/nmm	Li4XZ2	0.008	0.725
Li24Se2S6I6Br2	Pma2	Li3XZ	0.089	0.626
Li32S8I12Cl4	Cm	Li4XZ2	0.062	0.585
Li16S2I6Cl2O2	P4mm	Li4XZ2	0.091	0.872
Li24Se2Br6Cl2O6	Cmmm	Li3XZ	0.097	0.667
Li24S2Br4Cl4O6	Pmma	Li3XZ	0.055	0.767
Li32S6Cl16O2	Cmcm	Li4XZ2	0.085	0.825
Li14S4I2Br4	P4/nmm	Li7X2Z3	0.096	0.582
Li16Se1Br2Cl6O3	P4mm	Li4XZ2	0.07	0.624
Li32I16O8	I4/mmm	Li4XZ2	0.013	0.82

Li16S3I2Br6O1	P4mm	Li4XZ2	0.091	0.571
Li32S8I8Cl8	Cm	Li4XZ2	0.059	0.573
Li24Se4I6Br2O4	Cmm2	Li3XZ	0.095	0.712
Li24S4I2Cl6O4	Pmm2	Li3XZ	0.095	0.78
Li32Se2Br16O6	Cmcm	Li4XZ2	0.048	0.523
Li14I4Br2O4	P4mm	Li7X2Z3	0.031	0.521
Li32Cl12O8F4	P-4m2	Li4XZ2	0.036	0.862
Li16I6Br2O4	P4/mmm	Li4XZ2	0.015	0.652
Li24S6I6Cl2O2	Cmcm	Li3XZ	0.079	0.668
Li24Se4I6Cl2O4	Amm2	Li3XZ	0.095	0.65
Li16Cl6O4F2	P4/mmm	Li4XZ2	0.055	0.718
Li16S2Br4Cl4O2	P4mm	Li4XZ2	0.095	0.762
Li32Br4O8F12	Cm	Li4XZ2	0.084	0.699
Li24S8I4Br4	P4/mmm	Li3XZ	0.091	0.674
Li32Te8I8Cl8	Cm	Li4XZ2	0.099	0.667
Li16Se1I6Br2O3	P4mm	Li4XZ2	0.068	0.577
Li16S1I6Br2O3	P4mm	Li4XZ2	0.059	0.669
Li16S2I6Cl2O2	P4mm	Li4XZ2	0.085	0.68
Li16Se1I6Cl2O3	P4mm	Li4XZ2	0.07	0.733
Li16Br4Cl4O4	P4mm	Li4XZ2	0	0.689
Li16S1I4Cl4O3	P4mm	Li4XZ2	0.067	0.804
Li16Te1Br2Cl6O3	P4mm	Li4XZ2	0.09	0.634
Li24Se4I8O4	P4/mmm	Li3XZ	0.096	0.709
Li14Br2Cl4O4	P4/mmm	Li7X2Z3	0	0.765
Li16S4I4Br4	I4mm	Li4XZ2	0.086	0.646
Li14Se2S2I4Br2	I4mm	Li7X2Z3	0.099	0.671
Li24S2Br6O6F2	Pmm2	Li3XZ	0.086	0.828
Li16S2Br6Cl2O2	P4/mmm	Li4XZ2	0.096	0.576
Li24S2Br2Cl6O6	Pma2	Li3XZ	0.054	0.762
Li16S2I2Br6O2	P4mm	Li4XZ2	0.084	0.604
Li32Br12Cl4O8	P4mm	Li4XZ2	0	0.609
Li16Se1I2Br6O3	P4mm	Li4XZ2	0.072	0.651
Li9S2I2Br1O1	P4/mmm	Li3XZ	0.097	0.625
Li14Se2S2I4Br2	P4mm	Li7X2Z3	0.096	0.589
Li24S2Br6O6F2	Cmcm	Li3XZ	0.097	0.8
Li24Se2Br6Cl2O6	Cmme	Li3XZ	0.064	0.559
Li16I4Br4O4	P4/mmm	Li4XZ2	0.014	0.564
Li24S6Br4Cl4O2	Ama2	Li3XZ	0.078	0.725
Li24S4I8O4	P4_2/mmc	Li3XZ	0.082	0.6
Li24S6I2Br6O2	Pma2	Li3XZ	0.095	0.73
Li16S1I6Cl2O3	P4mm	Li4XZ2	0.072	0.752
Li14Se2S2I6	P4/nmm	Li7X2Z3	0.085	0.739
Li24S8I6Cl2	P4/mmm	Li3XZ	0.094	0.543

Li32S8I16	I4/mmm	Li4XZ2	0.062	0.814
Li16S1I4Cl4O3	P4mm	Li4XZ2	0.075	0.518
Li14S2I2Br4O2	P4mm	Li7X2Z3	0.088	0.712
Li16Se1I2Br6O3	P4mm	Li4XZ2	0.067	0.58
Li16S1Br2Cl6O3	P4mm	Li4XZ2	0.057	0.761
Li24S2Cl6O6F2	P222_1	Li3XZ	0.089	0.822
Li24S6I4Cl4O2	Pmm2	Li3XZ	0.097	0.854
Li24Se4S4I4Cl4	C2	Li3XZ	0.082	0.632
Li24Se2I6Br2O6	Cmme	Li3XZ	0.08	0.66
Li16I4Br4O4	P4mm	Li4XZ2	0.013	0.776
Li24Cl4O8F4	Pm-3m	Li3XZ	0.086	0.552
Li16Se1I4Cl4O3	P4mm	Li4XZ2	0.084	0.776
Li24S4Br8O4	P4/mmm	Li3XZ	0.096	0.569
Li24Se4I4Br4O4	Pmm2	Li3XZ	0.099	0.834
Li32Te8I12Cl4	P1	Li4XZ2	0.07	0.773
Li24Se2I4Br4O6	Cmm2	Li3XZ	0.071	0.825
Li24Se4I4Cl4O4	Cm	Li3XZ	0.084	0.653
Li24I6Br2O8	Im-3m	Li3XZ	0.074	0.684
Li16S1Br6Cl2O3	P4mm	Li4XZ2	0.062	0.774
Li24S4Br6Cl2O4	Pm	Li3XZ	0.069	0.791
Li24S2I2Br6O6	Amm2	Li3XZ	0.068	0.795
Li24S2I4Br4O6	Amm2	Li3XZ	0.074	0.659
Li32S6Br16O2	Cmcm	Li4XZ2	0.075	0.811
Li24S2Br4Cl4O6	Amm2	Li3XZ	0.068	0.656
Li32I4Br12O8	Cm	Li4XZ2	0.005	0.596
Li16Br2Cl6O4	P4/nmm	Li4XZ2	0	0.69
Li16I2Br6O4	P4/nmm	Li4XZ2	0.006	0.607
Li16Cl6O4F2	P4/nmm	Li4XZ2	0.054	0.666
Li14S2I4Cl2O2	P4mm	Li7X2Z3	0.094	0.764
Li16Se1Br6Cl2O3	P4/mmm	Li4XZ2	0.089	0.697
Li16Cl4O4F4	P4mm	Li4XZ2	0.097	0.6
Li24Se2I6Br2O6	Pmm2	Li3XZ	0.075	0.626
Li16Se3S1I6Br2	P4mm	Li4XZ2	0.096	0.622
Li24Se2I4Br4O6	Pm	Li3XZ	0.084	0.75
Li24S4I6Br2O4	Ama2	Li3XZ	0.079	0.799
Li16S1I2Cl6O3	P4mm	Li4XZ2	0.074	0.576
Li24S2Br6O6F2	Cmme	Li3XZ	0.091	0.648
Li16Te1Br6Cl2O3	P4mm	Li4XZ2	0.087	0.742
Li16Se1Br4Cl4O3	P4mm	Li4XZ2	0.071	0.784
Li24Te2S6I4Br4	Ama2	Li3XZ	0.093	0.58
Li16Se1Br8O3	P4/mmm	Li4XZ2	0.084	0.652
Li16Se1I2Cl6O3	P4mm	Li4XZ2	0.078	0.712
Li24S4Br2Cl6O4	P4/nmm	Li3XZ	0.083	0.697

Li32Br12Cl4O8	Cm	Li4XZ2	0	0.502
Li16S4I6Cl2	P4mm	Li4XZ2	0.089	0.756
Li16S4I4Br4	P4mm	Li4XZ2	0.084	0.585
Li32Se4S4Br16	P4_2/mmc	Li4XZ2	0.087	0.666
Li16I4Br4O4	P4mm	Li4XZ2	0.011	0.545
Li24Se4I2Cl6O4	Ama2	Li3XZ	0.097	0.59
Li16Se1Br4Cl4O3	P4mm	Li4XZ2	0.073	0.54
Li24S4I6Br2O4	Pmm2	Li3XZ	0.092	0.692
Li24Se2S6I6Br2	Pmm2	Li3XZ	0.091	0.681
Li32I8O8F8	Cm	Li4XZ2	0.097	0.724
Li32Se8I12Br4	Cm	Li4XZ2	0.06	0.712
Li16Se3S1I6Br2	P4/mmm	Li4XZ2	0.096	0.881
Li32Br4Cl12O8	P4mm	Li4XZ2	0	0.65
Li16I2Br6O4	P4/mmm	Li4XZ2	0.007	0.894
Li16Se3S1I6Br2	P4mm	Li4XZ2	0.094	0.651
Li16S1I6Br2O3	P4mm	Li4XZ2	0.052	0.637
Li16S3I2Br6O1	P4mm	Li4XZ2	0.092	0.789
Li16S1I6Cl2O3	P4/mmm	Li4XZ2	0.076	0.719
Li24Se4I4Br4O4	R3m	Li3XZ	0.092	0.882
Li32Br12Cl4O8	Cm	Li4XZ2	0	0.598
Li16S1I2Br6O3	P4mm	Li4XZ2	0.056	0.787
Li16S1I6Br2O3	P4mm	Li4XZ2	0.053	0.835
Li24S4I4Br4O4	C2	Li3XZ	0.08	0.604
Li24S6I4Cl4O2	Pm	Li3XZ	0.08	0.652
Li24S8I4Br4	P4/mmm	Li3XZ	0.09	0.767
Li14Se2S2I6	I4mm	Li7X2Z3	0.085	0.783
Li16S1I4Br4O3	P4mm	Li4XZ2	0.061	0.654
Li24Se2I2Br6O6	Pma2	Li3XZ	0.065	0.648
Li16Se1I4Cl4O3	P4mm	Li4XZ2	0.073	0.51
Li16S4I6Cl2	P4/mmm	Li4XZ2	0.089	0.666
Li24Te2I6Br2O6	Pma2	Li3XZ	0.088	0.732
Li24Br6O8F2	P4/mmm	Li3XZ	0.066	0.557
Li24S4I2Br6O4	C2/c	Li3XZ	0.078	0.803
Li16S1I4Cl4O3	P4mm	Li4XZ2	0.065	0.622
Li16S3I4Br4O1	P4mm	Li4XZ2	0.091	0.841
Li14S2I4Br2O2	P4mm	Li7X2Z3	0.083	0.56
Li24S2Br6Cl2O6	Pma2	Li3XZ	0.055	0.665
Li24S4I6Br2O4	P2	Li3XZ	0.078	0.522
Li32S4Br16O4	P4_2/mmc	Li4XZ2	0.064	0.764
Li16Se1I2Br6O3	P4/mmm	Li4XZ2	0.089	0.607
Li32S8I4Br12	P4mm	Li4XZ2	0.093	0.564
Li24S2I6Br2O6	Amm2	Li3XZ	0.079	0.532
Li24S2Cl8O6	Im-3m	Li3XZ	0.061	0.552

Li ₂₄ Se ₄ I ₂ Br ₆ O ₄	C2/c	Li ₃ XZ	0.096	0.785
Li ₁₆ S ₁ Cl ₈ O ₃	P4/mmm	Li ₄ XZ ₂	0.067	0.793
Li ₁₆ S ₁ Br ₂ Cl ₆ O ₃	P4mm	Li ₄ XZ ₂	0.058	0.589
Li ₂₄ S ₂ I ₆ Cl ₂ O ₆	Cmcm	Li ₃ XZ	0.087	0.571
Li ₂₄ Se ₆ I ₆ Br ₂ O ₂	Pma2	Li ₃ XZ	0.099	0.799
Li ₂₄ S ₂ I ₄ Cl ₄ O ₆	P4 ₂ /mcm	Li ₃ XZ	0.091	0.667
Li ₂₄ S ₆ I ₆ Cl ₂ O ₂	P222 ₁	Li ₃ XZ	0.096	0.646
Li ₂₄ S ₄ Cl ₆ O ₄ F ₂	Pm	Li ₃ XZ	0.094	0.519
Li ₂₄ S ₂ Br ₂ Cl ₆ O ₆	Cmcm	Li ₃ XZ	0.05	0.57
Li ₁₆ S ₃ I ₄ Br ₄ O ₁	P4mm	Li ₄ XZ ₂	0.089	0.624
Li ₁₆ Se ₁ I ₆ Br ₂ O ₃	P4mm	Li ₄ XZ ₂	0.065	0.675
Li ₉ I ₂ Cl ₁ O ₃	P4/mmm	Li ₃ XZ	0.063	0.55
Li ₂₄ S ₆ I ₆ Cl ₂ O ₂	Pma2	Li ₃ XZ	0.086	0.744
Li ₂₄ Te ₂ Br ₄ Cl ₄ O ₆	P4mm	Li ₃ XZ	0.086	0.567
Li ₁₆ Te ₁ Br ₂ Cl ₆ O ₃	P4mm	Li ₄ XZ ₂	0.093	0.756
Li ₂₄ Se ₄ I ₆ Br ₂ O ₄	C2/c	Li ₃ XZ	0.095	0.681
Li ₁₆ S ₂ I ₆ Br ₂ O ₂	P4mm	Li ₄ XZ ₂	0.074	0.854
Li ₁₆ S ₁ Br ₆ Cl ₂ O ₃	P4mm	Li ₄ XZ ₂	0.057	0.556
Li ₃₂ I ₄ Br ₁₂ O ₈	P4mm	Li ₄ XZ ₂	0.008	0.64
Li ₉ S ₁ I ₃ O ₂	P4/mmm	Li ₃ XZ	0.098	0.752
Li ₃₂ I ₁₂ Cl ₄ O ₈	Cm	Li ₄ XZ ₂	0.019	0.848
Li ₁₄ Br ₄ O ₄ F ₂	P4mm	Li ₇ X ₂ Z ₃	0.081	0.76
Li ₁₆ Te ₁ I ₆ Br ₂ O ₃	P4mm	Li ₄ XZ ₂	0.083	0.671
Li ₂₄ Se ₂ I ₆ Cl ₂ O ₆	P222 ₁	Li ₃ XZ	0.085	0.575
Li ₁₆ S ₂ Br ₄ Cl ₄ O ₂	P4mm	Li ₄ XZ ₂	0.095	0.55
Li ₁₆ Cl ₆ O ₄ F ₂	P4/mmm	Li ₄ XZ ₂	0.054	0.741
Li ₃₂ Te ₆ S ₂ I ₁₆	Cmcm	Li ₄ XZ ₂	0.096	0.61
Li ₁₆ Se ₁ S ₃ I ₆ Br ₂	P4mm	Li ₄ XZ ₂	0.083	0.698
Li ₁₆ Se ₁ I ₄ Br ₄ O ₃	P4mm	Li ₄ XZ ₂	0.071	0.639
Li ₁₄ S ₂ I ₆ O ₂	I4mm	Li ₇ X ₂ Z ₃	0.077	0.834
Li ₃₂ S ₂ Br ₁₆ O ₆	Cmcm	Li ₄ XZ ₂	0.033	0.819
Li ₂₄ Cl ₆ O ₈ F ₂	P4/mmm	Li ₃ XZ	0.044	0.654
Li ₃₂ Br ₄ Cl ₁₂ O ₈	Pmm2	Li ₄ XZ ₂	0	0.737
Li ₁₆ I ₄ Cl ₄ O ₄	P4/mmm	Li ₄ XZ ₂	0.008	0.61
Li ₃₂ Se ₈ I ₈ Cl ₈	Cm	Li ₄ XZ ₂	0.073	0.662
Li ₂₄ Se ₂ Br ₄ Cl ₄ O ₆	Ama2	Li ₃ XZ	0.071	0.857
Li ₁₆ I ₆ O ₄ F ₂	P4mm	Li ₄ XZ ₂	0.098	0.595
Li ₃₂ Br ₈ Cl ₈ O ₈	Pmm2	Li ₄ XZ ₂	0	0.755
Li ₁₆ Cl ₆ O ₄ F ₂	P4mm	Li ₄ XZ ₂	0.054	0.722
Li ₂₄ Se ₂ S ₆ I ₆ Br ₂	Cmmm	Li ₃ XZ	0.089	0.642
Li ₁₄ Cl ₄ O ₄ F ₂	P4/mmm	Li ₇ X ₂ Z ₃	0.067	0.576
Li ₃₂ Se ₄ Cl ₁₆ O ₄	P4 ₂ /mmc	Li ₄ XZ ₂	0.099	0.782
Li ₂₄ Se ₄ S ₄ I ₈	P4/mmm	Li ₃ XZ	0.086	0.572

Li ₂₄ S ₄ Br ₂ Cl ₆ O ₄	Pm	Li ₃ XZ	0.072	0.711
Li ₂₄ Se ₆ I ₆ Br ₂ O ₂	Cmcm	Li ₃ XZ	0.088	0.615
Li ₃₂ Se ₈ I ₂ Cl ₄	P4mm	Li ₄ XZ ₂	0.096	0.609
Li ₁₆ I ₆ Br ₂ O ₄	P4mm	Li ₄ XZ ₂	0.014	0.571
Li ₁₆ S ₄ I ₆ Br ₂	P4mm	Li ₄ XZ ₂	0.074	0.515
Li ₁₆ S ₁ Br ₆ Cl ₂ O ₃	P4mm	Li ₄ XZ ₂	0.054	0.627
Li ₉ S ₁ I ₁ Br ₂ O ₂	P4mm	Li ₃ XZ	0.086	0.805
Li ₂₄ S ₄ Cl ₈ O ₄	Fm-3m	Li ₃ XZ	0.081	0.698
Li ₂₄ Se ₂ I ₆ Br ₂ O ₆	Pma2	Li ₃ XZ	0.089	0.694
Li ₃₂ Te ₂ I ₁₆ O ₆	P4/mmm	Li ₄ XZ ₂	0.074	0.595
Li ₃₂ I ₄ Cl ₁₂ O ₈	Cm	Li ₄ XZ ₂	0.005	0.702
Li ₂₄ Se ₂ Br ₈ O ₆	Im-3m	Li ₃ XZ	0.076	0.566
Li ₂₄ S ₄ I ₄ Cl ₄ O ₄	Cm	Li ₃ XZ	0.076	0.61
Li ₁₆ Se ₂ I ₈ O ₂	P4/nmm	Li ₄ XZ ₂	0.095	0.687
Li ₁₆ S ₃ Br ₈ O ₁	P4/mmm	Li ₄ XZ ₂	0.097	0.813
Li ₂₄ S ₆ I ₆ Br ₂ O ₂	Cmcm	Li ₃ XZ	0.072	0.568
Li ₁₄ Br ₄ O ₄ F ₂	P4/nmm	Li ₇ X ₂ Z ₃	0.059	0.827
Li ₃₂ Te ₂ Cl ₁₆ O ₆	Cmcm	Li ₄ XZ ₂	0.079	0.771
Li ₁₆ Se ₁ S ₃ I ₄ Br ₄	P4mm	Li ₄ XZ ₂	0.092	0.662
Li ₃₂ Te ₄ I ₁₆ O ₄	Cmmm	Li ₄ XZ ₂	0.095	0.646
Li ₁₆ Se ₁ I ₆ Br ₂ O ₃	P4mm	Li ₄ XZ ₂	0.074	0.668
Li ₁₆ S ₂ I ₄ Cl ₄ O ₂	P4mm	Li ₄ XZ ₂	0.094	0.709
Li ₃₂ S ₈ I ₂ Cl ₄	Cm	Li ₄ XZ ₂	0.057	0.652
Li ₁₆ Br ₂ Cl ₆ O ₄	P4/mmm	Li ₄ XZ ₂	0	0.624
Li ₂₄ S ₂ I ₆ Br ₂ O ₆	P222_1	Li ₃ XZ	0.07	0.728
Li ₂₄ Br ₄ O ₈ F ₄	P4/mmm	Li ₃ XZ	0.1	0.807
Li ₁₆ Se ₁ I ₂ Cl ₆ O ₃	P4mm	Li ₄ XZ ₂	0.081	0.805
Li ₁₆ S ₁ Br ₂ Cl ₆ O ₃	P4/mmm	Li ₄ XZ ₂	0.068	0.654
Li ₂₄ S ₄ I ₆ Br ₂ O ₄	Pm	Li ₃ XZ	0.075	0.576
Li ₂₄ S ₆ Br ₆ Cl ₂ O ₂	Pma2	Li ₃ XZ	0.086	0.826
Li ₁₆ S ₁ Br ₄ Cl ₄ O ₃	P4/mmm	Li ₄ XZ ₂	0.069	0.548
Li ₁₄ Br ₄ Cl ₂ O ₄	I4/mmm	Li ₇ X ₂ Z ₃	0	0.63
Li ₁₆ Se ₁ S ₃ I ₆ Br ₂	P4/mmm	Li ₄ XZ ₂	0.083	0.549
Li ₃₂ Te ₆ Se ₂ I ₁₆	Cmcm	Li ₄ XZ ₂	0.099	0.543
Li ₂₄ S ₆ I ₂ Br ₆ O ₂	Cmmm	Li ₃ XZ	0.1	0.701
Li ₂₄ S ₂ Cl ₆ O ₆ F ₂	Cmcm	Li ₃ XZ	0.079	0.667
Li ₂₄ S ₆ I ₈ O ₂	P4/mmm	Li ₃ XZ	0.079	0.702
Li ₂₄ S ₂ Cl ₄ O ₆ F ₄	Pm	Li ₃ XZ	0.097	0.526
Li ₃₂ S ₈ I ₄ Cl ₁₂	Cm	Li ₄ XZ ₂	0.061	0.631
Li ₁₄ S ₂ I ₄ Br ₂ O ₂	P4/mmm	Li ₇ X ₂ Z ₃	0.098	0.709
Li ₁₆ Se ₂ S ₂ I ₄ Br ₄	P4mm	Li ₄ XZ ₂	0.1	0.561
Li ₂₄ Se ₆ I ₆ Cl ₂ O ₂	Cmcm	Li ₃ XZ	0.094	0.716
Li ₁₆ I ₄ Cl ₄ O ₄	P4mm	Li ₄ XZ ₂	0.019	0.805

Li ₂₄ Se ₂ I ₄ Cl ₄ O ₆	Pmm2	Li ₃ XZ	0.08	0.769
Li ₁₄ S ₄ I ₄ Br ₂	I4/mmm	Li ₇ X ₂ Z ₃	0.085	0.571
Li ₃₂ Te ₈ I ₄ Br ₁₂	Cm	Li ₄ XZ ₂	0.092	0.682
Li ₂₄ S ₂ Br ₆ O ₆ F ₂	P222_1	Li ₃ XZ	0.093	0.774
Li ₂₄ S ₄ I ₆ Br ₂ O ₄	P4/nmm	Li ₃ XZ	0.094	0.585
Li ₂₄ S ₄ Br ₄ Cl ₄ O ₄	C2	Li ₃ XZ	0.064	0.796
Li ₂₄ S ₄ I ₄ Br ₄ O ₄	Pmm2	Li ₃ XZ	0.078	0.767
Li ₂₄ S ₄ Br ₈ O ₄	P4/mmm	Li ₃ XZ	0.079	0.585
Li ₂₄ Te ₂ Br ₂ Cl ₆ O ₆	Pmm2	Li ₃ XZ	0.088	0.539
Li ₁₄ S ₂ Br ₆ O ₂	P4/mmm	Li ₇ X ₂ Z ₃	0.094	0.758
Li ₁₆ Se ₁ I ₄ Br ₄ O ₃	P4mm	Li ₄ XZ ₂	0.075	0.798
Li ₂₄ Se ₄ I ₄ Br ₄ O ₄	C2	Li ₃ XZ	0.084	0.686
Li ₂₄ Se ₄ I ₆ Cl ₂ O ₄	P2	Li ₃ XZ	0.098	0.709
Li ₁₆ Se ₁ I ₆ Cl ₂ O ₃	P4mm	Li ₄ XZ ₂	0.075	0.702
Li ₃₂ S ₈ I ₄ Cl ₁₂	P1	Li ₄ XZ ₂	0.058	0.68
Li ₃₂ I ₈ Br ₈ O ₈	Cm	Li ₄ XZ ₂	0.013	0.77
Li ₂₄ S ₂ Br ₆ O ₆ F ₂	Cmmm	Li ₃ XZ	0.09	0.57
Li ₂₄ Se ₂ I ₄ Br ₄ O ₆	Ama2	Li ₃ XZ	0.084	0.764
Li ₃₂ S ₈ I ₈ Br ₈	Cm	Li ₄ XZ ₂	0.055	0.756
Li ₁₆ Se ₁ Br ₆ Cl ₂ O ₃	P4mm	Li ₄ XZ ₂	0.068	0.693
Li ₂₄ S ₄ Br ₆ Cl ₂ O ₄	P2	Li ₃ XZ	0.075	0.675
Li ₂₄ Se ₂ S ₆ I ₆ Cl ₂	Cmmm	Li ₃ XZ	0.087	0.552
Li ₁₆ Se ₁ S ₃ I ₆ Cl ₂	P4mm	Li ₄ XZ ₂	0.097	0.554
Li ₁₄ I ₄ Br ₂ O ₄	P4/mmm	Li ₇ X ₂ Z ₃	0.045	0.812
Li ₁₆ Br ₆ O ₄ F ₂	P4/nmm	Li ₄ XZ ₂	0.043	0.689
Li ₁₆ Te ₁ I ₂ Br ₆ O ₃	P4mm	Li ₄ XZ ₂	0.086	0.568
Li ₂₄ Se ₂ Br ₆ Cl ₂ O ₆	Pmm2	Li ₃ XZ	0.072	0.676
Li ₂₄ S ₂ I ₄ Cl ₄ O ₆	Pmma	Li ₃ XZ	0.084	0.75
Li ₁₄ I ₄ Cl ₂ O ₄	I4/mmm	Li ₇ X ₂ Z ₃	0.012	0.553
Li ₉ S ₁ I ₁ Br ₂ O ₂	P4/mmm	Li ₃ XZ	0.096	0.795
Li ₁₆ Se ₁ S ₃ I ₂ Br ₆	P4mm	Li ₄ XZ ₂	0.1	0.693
Li ₁₆ S ₄ I ₂ Br ₆	P4mm	Li ₄ XZ ₂	0.092	0.76
Li ₂₄ S ₄ I ₄ Br ₄ O ₄	P4mm	Li ₃ XZ	0.094	0.66
Li ₂₄ Br ₄ Cl ₄ O ₈	P4_2/mmc	Li ₃ XZ	0.008	0.577
Li ₁₆ I ₂ Cl ₆ O ₄	P4mm	Li ₄ XZ ₂	0.008	0.617
Li ₁₆ Se ₁ I ₆ Cl ₂ O ₃	P4mm	Li ₄ XZ ₂	0.085	0.762
Li ₁₆ S ₁ Br ₄ Cl ₄ O ₃	P4mm	Li ₄ XZ ₂	0.061	0.544
Li ₂₄ S ₄ I ₄ Br ₄ O ₄	P4/nmm	Li ₃ XZ	0.096	0.577
Li ₂₄ S ₈ I ₆ Br ₂	P4/mmm	Li ₃ XZ	0.08	0.51
Li ₂₄ S ₂ Cl ₈ O ₆	P4/mmm	Li ₃ XZ	0.055	0.606
Li ₂₄ S ₄ I ₄ Br ₄ O ₄	P4mm	Li ₃ XZ	0.094	0.776
Li ₁₆ S ₂ Br ₆ Cl ₂ O ₂	P4mm	Li ₄ XZ ₂	0.092	0.688
Li ₁₆ Se ₃ S ₁ I ₆ Br ₂	P4mm	Li ₄ XZ ₂	0.096	0.596

Li ₂₄ S ₂ Br ₄ Cl ₄ O ₆	Cmmm	Li ₃ XZ	0.069	0.609
Li ₃₂ I ₈ O ₈ F ₈	Cm	Li ₄ XZ ₂	0.096	0.654
Li ₁₆ I ₆ Br ₂ O ₄	P4/mmm	Li ₄ XZ ₂	0.015	0.721
Li ₂₄ S ₄ Br ₄ Cl ₄ O ₄	Cm	Li ₃ XZ	0.062	0.81
Li ₂₄ Se ₂ Br ₄ Cl ₄ O ₆	Cmm2	Li ₃ XZ	0.073	0.614
Li ₃₂ S ₈ I ₁₂ F ₄	Cm	Li ₄ XZ ₂	0.096	0.765
Li ₃₂ I ₁₂ Br ₄ O ₈	P1	Li ₄ XZ ₂	0.013	0.655
Li ₁₆ S ₂ I ₆ Br ₂ O ₂	P4mm	Li ₄ XZ ₂	0.078	0.88
Li ₁₆ S ₂ I ₂ Br ₆ O ₂	P4/mmm	Li ₄ XZ ₂	0.088	0.728
Li ₃₂ I ₈ Br ₈ O ₈	Pmm2	Li ₄ XZ ₂	0.012	0.696

Table S3. List of candidate solid state reactions for $Pm\bar{3}m$ Li_3OCl inverse-perovskite compound based on a data-driven approach in Reference 76 of the main text. Reactions are summarized with their number of competing phases that formed aside from the target phase, nucleation barrier based on classical nucleation theory, reaction enthalpy, and multi-objective decision-making metric called TOPSIS score. Compound tags in parenthesis indicate the Materials Project ID.

Number of competing phases	Nucleation barrier / a.u.	Reaction summary	Enthalpy / eV	TOPSIS score
3	0.785	0.5 C(mp-569304) + -0.5 CO ₂ (mp-20066) + 1.0 Li ₂ O ₂ (mp-841) + 1.0 LiCl(mp-1185319)	-0.397	0.909
3	0.789	-0.48 CO ₂ (mp-20066) + 0.98 Li ₂ O ₂ (mp-841) + 0.04 LiC ₁₂ (mp-1021323) + 1.0 LiCl(mp-1185319)	-0.404	0.909
3	1.2	-24.0 CO ₂ (mp-20066) + 2.0 LiC ₁₂ (mp-1021323) + 1.0 LiCl(mp-1185319) + 24.5 O ₂ (mp-12957)	-24.337	0.87
4	0.677	1.0 ClO ₂ (mp-23207) + 1.5 Li ₂ O(mp-1960) + -1.25 O ₂ (mp-12957)	0.11	0.86
5	0.315	-1.7143 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 1.4286 Li ₂ O(mp-1960) + 0.1429 LiC ₁₂ (mp-1021323)	-1.566	0.816
5	0.316	1.75 C(mp-569304) + -1.75 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 1.5 Li ₂ O(mp-1960)	-1.514	0.816
5	0.33	-1.2245 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 1.449 Li ₂ O(mp-1960) + 0.102 LiC ₁₂ (mp-1021323)	-1.132	0.816
5	0.33	1.25 C(mp-569304) + -1.25 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 1.5 Li ₂ O(mp-1960)	-1.095	0.816
5	0.611	2.0 C(mp-569304) + -2.0 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 1.5 Li ₂ O ₂ (mp-841)	-1.697	0.808
5	0.611	-1.92 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 1.42 Li ₂ O ₂ (mp-841) + 0.16 LiC ₁₂ (mp-1021323)	-1.723	0.808
6	0.312	-1.9592 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 1.4184 Li ₂ O(mp-1960) + 0.1633 LiC ₁₂ (mp-1021323)	-1.812	0.767
6	0.312	2.0 C(mp-569304) + -2.0 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 1.5 Li ₂ O(mp-1960)	-1.753	0.767
6	0.447	0.5 Cl ₂ O ₇ (mp-31050) + 1.5 Li ₂ O(mp-1960) + -2.0 O ₂ (mp-12957)	0.175	0.764
6	0.502	1.0 ClO ₃ (mp-22869) + 1.5 Li ₂ O(mp-1960) + -1.75 O ₂ (mp-12957)	0.173	0.762
6	0.606	2.75 C(mp-569304) + -2.75 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 1.5 Li ₂ O ₂ (mp-841)	-2.355	0.759
6	0.606	-2.64 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 1.39 Li ₂ O ₂ (mp-841) + 0.22 LiC ₁₂ (mp-1021323)	-2.39	0.759
6	0.607	2.5 C(mp-569304) + -2.5 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 1.5 Li ₂ O ₂ (mp-841)	-2.116	0.759

6	0.607	-2.4 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 1.4 Li ₂ O ₂ (mp-841) + 0.2 LiC ₁₂ (mp-1021323)	-2.148	0.759
6	0.677	0.5 Cl ₂ O ₇ (mp-31050) + 1.5 Li ₂ O ₂ (mp-841) + -2.75 O ₂ (mp-12957)	0.296	0.756
6	0.698	1.0 ClO ₃ (mp-22869) + 1.5 Li ₂ O ₂ (mp-841) + -2.5 O ₂ (mp-12957)	0.294	0.755
6	0.752	1.0 ClO ₂ (mp-23207) + 1.5 Li ₂ O ₂ (mp-841) + -2.0 O ₂ (mp-12957)	0.231	0.753
5	2.965	-3.1429 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 1.4286 Li ₂ CO ₃ (mp-3054) + 0.1429 LiC ₁₂ (mp-1021323)	-0.847	0.615
5	2.97	1.75 C(mp-569304) + -3.25 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 1.5 Li ₂ CO ₃ (mp-3054)	-0.759	0.615
5	3.017	-2.6735 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 1.449 Li ₂ CO ₃ (mp-3054) + 0.102 LiC ₁₂ (mp-1021323)	-0.402	0.61
5	3.026	1.25 C(mp-569304) + -2.75 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 1.5 Li ₂ CO ₃ (mp-3054)	-0.34	0.609
2	3.724	1.0 Li ₂ O ₂ (mp-841) + 1.0 LiCl(mp-1185319) + -0.5 O ₂ (mp-12957)	0.085	0.598
6	2.95	-3.3776 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 1.4184 Li ₂ CO ₃ (mp-3054) + 0.1633 LiC ₁₂ (mp-1021323)	-1.098	0.587
6	2.954	2.0 C(mp-569304) + -3.5 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 1.5 Li ₂ CO ₃ (mp-3054)	-0.997	0.587
6	3.38	-1.5 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 1.5 Li ₂ CO ₃ (mp-3054) + -2.0 O ₂ (mp-12957)	0.93	0.543
6	3.507	-1.5 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 1.5 Li ₂ CO ₃ (mp-3054) + -1.75 O ₂ (mp-12957)	0.928	0.529
6	3.837	-1.5 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 1.5 Li ₂ CO ₃ (mp-3054) + -1.25 O ₂ (mp-12957)	0.865	0.493
2	6.371	-1.0 CO ₂ (mp-20066) + 1.0 Li ₂ CO ₃ (mp-3054) + 1.0 LiCl(mp-1185319)	0.508	0.35
7	7.901	-36.0 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 3.0 LiC ₁₂ (mp-1021323) + 34.75 O ₂ (mp-12957)	-36.336	0
7	7.901	-36.0 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 3.0 LiC ₁₂ (mp-1021323) + 35.0 O ₂ (mp-12957)	-36.339	0
7	7.901	-36.0 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 3.0 LiC ₁₂ (mp-1021323) + 35.5 O ₂ (mp-12957)	-36.401	0

Table S4. List of candidate solid state reactions for $I4/mmm$ Li_4OBr_2 inverse-perovskite compound based on a data-driven approach in Reference 76 of the main text. Reactions are summarized with their number of competing phases that formed aside from the target phase, nucleation barrier based on classical nucleation theory, reaction enthalpy, and multi-objective decision-making metric called TOPSIS score. Compound tags in parenthesis indicate the Materials Project ID.

Number of competing phases	Nucleation barrier / a.u.	Reaction summary	Enthalpy / eV	TOPSIS score
2	1.224	0.5 C(mp-569304) + -0.5 CO ₂ (mp-20066) + 1.0 Li ₂ O ₂ (mp-841) + 2.0 LiBr(mp-976280)	-0.289	0.894
2	1.237	-0.48 CO ₂ (mp-20066) + 0.98 Li ₂ O ₂ (mp-841) + 2.0 LiBr(mp-976280) + 0.04 LiC ₁₂ (mp-1021323)	-0.293	0.894
2	10.54	1.0 Li ₂ O ₂ (mp-841) + 2.0 LiBr(mp-976280) + -0.5 O ₂ (mp-12957)	0.056	0.894
2	17.064	-1.0 CO ₂ (mp-20066) + 1.0 Li ₂ CO ₃ (mp-3054) + 2.0 LiBr(mp-976280)	0.358	0.894
4	0.808	1.0 Br ₂ O ₃ (mp-28933) + 2.0 Li ₂ O(mp-1960) + -2.0 O ₂ (mp-12957)	0.136	0.804
4	0.827	1.0 Br ₂ O ₃ (mp-28933) + 2.0 Li ₂ O ₂ (mp-841) + -3.0 O ₂ (mp-12957)	0.251	0.804
4	0.901	-24.0 CO ₂ (mp-20066) + 2.0 LiBr(mp-976280) + 2.0 LiC ₁₂ (mp-1021323) + 24.5 O ₂ (mp-12957)	-17.388	0.804
4	4.306	1.0 Br ₂ O ₃ (mp-28933) + -2.0 CO ₂ (mp-20066) + 2.0 Li ₂ CO ₃ (mp-3054) + -2.0 O ₂ (mp-12957)	0.855	0.804
5	0.339	1.0 Br ₂ O ₃ (mp-28933) + -1.9592 CO ₂ (mp-20066) + 1.9184 Li ₂ O(mp-1960) + 0.1633 LiC ₁₂ (mp-1021323)	-1.284	0.766
5	0.34	1.0 Br ₂ O ₃ (mp-28933) + 2.0 C(mp-569304) + -2.0 CO ₂ (mp-20066) + 2.0 Li ₂ O(mp-1960)	-1.241	0.766
5	0.616	1.0 Br ₂ O ₃ (mp-28933) + 3.0 C(mp-569304) + -3.0 CO ₂ (mp-20066) + 2.0 Li ₂ O ₂ (mp-841)	-1.815	0.766
5	0.617	1.0 Br ₂ O ₃ (mp-28933) + -2.88 CO ₂ (mp-20066) + 1.88 Li ₂ O ₂ (mp-841) + 0.24 LiC ₁₂ (mp-1021323)	-1.842	0.766
5	3.061	1.0 Br ₂ O ₃ (mp-28933) + -3.8776 CO ₂ (mp-20066) + 1.9184 Li ₂ CO ₃ (mp-3054) + 0.1633 LiC ₁₂ (mp-1021323)	-0.594	0.766
5	3.074	1.0 Br ₂ O ₃ (mp-28933) + 2.0 C(mp-569304) + -4.0 CO ₂ (mp-20066) + 2.0 Li ₂ CO ₃ (mp-3054)	-0.522	0.766
6	7.302	1.0 Br ₂ O ₃ (mp-28933) + -48.0 CO ₂ (mp-20066) + 4.0 LiC ₁₂ (mp-1021323) + 47.0 O ₂ (mp-12957)	-34.637	0.731
0	44,201.06	1.0 Li ₂ O(mp-1960) + 2.0 LiBr(mp-976280)	-0.002	0.269

Table S5. List of candidate solid state reactions for $P4/nmm$ $\text{Li}_8\text{O}_2\text{Cl}_3\text{Br}$ inverse-perovskite compound based on a data-driven approach in Reference 76 of the main text. Reactions are summarized with their number of competing phases that formed aside from the target phase, nucleation barrier based on classical nucleation theory, reaction enthalpy, and multi-objective decision-making metric called TOPSIS score. Compound tags in parenthesis indicate the Materials Project ID.

Number of competing phases	Nucleation barrier / a.u.	Reaction summary	Enthalpy / eV	TOPSIS score
3	0.305	-5.8776 $\text{CO}_2(\text{mp-20066}) + 1.7551 \text{Li}_2\text{O}(\text{mp-1960}) + 1.0 \text{LiBr}(\text{mp-976280}) + 0.4898 \text{LiC12}(\text{mp-1021323}) + 3.0 \text{LiClO}_4(\text{mp-30301})$	-1.601	0.973
3	0.607	0.5 $\text{Br}_2\text{O}_3(\text{mp-28933}) + -7.92 \text{CO}_2(\text{mp-20066}) + 3.0 \text{ClO}_3(\text{mp-22869}) + 3.67 \text{Li}_2\text{O}_2(\text{mp-841}) + 0.66 \text{LiC12}(\text{mp-1021323})$	-2.545	0.963
4	0.306	6.0 $\text{C}(\text{mp-569304}) + -6.0 \text{CO}_2(\text{mp-20066}) + 2.0 \text{Li}_2\text{O}(\text{mp-1960}) + 1.0 \text{LiBr}(\text{mp-976280}) + 3.0 \text{LiClO}_4(\text{mp-30301})$	-1.538	0.946
4	0.436	2.0 $\text{Li}_2\text{O}(\text{mp-1960}) + 1.0 \text{LiBr}(\text{mp-976280}) + 3.0 \text{LiClO}_4(\text{mp-30301}) + -6.0 \text{O}_2(\text{mp-12957})$	0.528	0.945
4	0.714	3.0 $\text{ClO}_2(\text{mp-23207}) + 3.5 \text{Li}_2\text{O}(\text{mp-1960}) + 1.0 \text{LiBr}(\text{mp-976280}) + -3.75 \text{O}_2(\text{mp-12957})$	0.116	0.936
4	0.9	-48.0 $\text{CO}_2(\text{mp-20066}) + 1.0 \text{LiBr}(\text{mp-976280}) + 4.0 \text{LiC12}(\text{mp-1021323}) + 3.0 \text{LiClO}_4(\text{mp-30301}) + 43.0 \text{O}_2(\text{mp-12957})$	-16.858	0.927
4	0.912	-7.6327 $\text{CO}_2(\text{mp-20066}) + 1.7551 \text{Li}_2\text{CO}_3(\text{mp-3054}) + 1.0 \text{LiBr}(\text{mp-976280}) + 0.4898 \text{LiC12}(\text{mp-1021323}) + 3.0 \text{LiClO}_4(\text{mp-30301})$	-1.286	0.926
5	0.317	-5.1429 $\text{CO}_2(\text{mp-20066}) + 3.0 \text{ClO}_3(\text{mp-22869}) + 3.2857 \text{Li}_2\text{O}(\text{mp-1960}) + 1.0 \text{LiBr}(\text{mp-976280}) + 0.4286 \text{LiC12}(\text{mp-1021323})$	-1.679	0.921
5	0.317	5.25 $\text{C}(\text{mp-569304}) + -5.25 \text{CO}_2(\text{mp-20066}) + 3.0 \text{ClO}_3(\text{mp-22869}) + 3.5 \text{Li}_2\text{O}(\text{mp-1960}) + 1.0 \text{LiBr}(\text{mp-976280})$	-1.624	0.921
5	0.333	-3.6735 $\text{CO}_2(\text{mp-20066}) + 3.0 \text{ClO}_2(\text{mp-23207}) + 3.3469 \text{Li}_2\text{O}(\text{mp-1960}) + 1.0 \text{LiBr}(\text{mp-976280}) + 0.3061 \text{LiC12}(\text{mp-1021323})$	-1.214	0.921
5	0.333	3.75 $\text{C}(\text{mp-569304}) + -3.75 \text{CO}_2(\text{mp-20066}) + 3.0 \text{ClO}_2(\text{mp-23207}) + 3.5 \text{Li}_2\text{O}(\text{mp-1960}) + 1.0 \text{LiBr}(\text{mp-976280})$	-1.175	0.921
5	0.387	0.5 $\text{Br}_2\text{O}_3(\text{mp-28933}) + 2.5 \text{Li}_2\text{O}(\text{mp-1960}) + 3.0 \text{LiClO}_4(\text{mp-30301}) + -7.0 \text{O}_2(\text{mp-12957})$	0.562	0.92
5	0.607	-6.72 $\text{CO}_2(\text{mp-20066}) + 1.72 \text{Li}_2\text{O}_2(\text{mp-841}) + 1.0 \text{LiBr}(\text{mp-976280}) + 0.56 \text{LiC12}(\text{mp-1021323}) + 3.0 \text{LiClO}_4(\text{mp-30301})$	-1.857	0.916
5	0.626	0.5 $\text{Br}_2\text{O}_3(\text{mp-28933}) + -0.9796 \text{CO}_2(\text{mp-20066}) + 2.4592 \text{Li}_2\text{O}(\text{mp-1960}) + 0.0816 \text{LiC12}(\text{mp-1021323}) + 3.0 \text{LiCl}(\text{mp-1185319})$	-0.317	0.916

5	0.633	0.5 Br ₂ O ₃ (mp-28933) + 1.0 C(mp-569304) + -1.0 CO ₂ (mp-20066) + 2.5 Li ₂ O(mp-1960) + 3.0 LiCl(mp-1185319)	-0.307	0.915
5	0.696	0.5 Br ₂ O ₃ (mp-28933) + 2.5 Li ₂ O ₂ (mp-841) + 3.0 LiClO ₄ (mp-30301) + -8.25 O ₂ (mp-12957)	0.634	0.913
5	0.946	-7.0204 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 3.3469 Li ₂ CO ₃ (mp-3054) + 1.0 LiBr(mp-976280) + 0.3061 LiC ₁₂ (mp-1021323)	-0.612	0.904
6	0.313	-5.8776 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 3.2551 Li ₂ O(mp-1960) + 1.0 LiBr(mp-976280) + 0.4898 LiC ₁₂ (mp-1021323)	-1.943	0.897
6	0.313	6.0 C(mp-569304) + -6.0 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 3.5 Li ₂ O(mp-1960) + 1.0 LiBr(mp-976280)	-1.879	0.897
6	0.313	0.5 Br ₂ O ₃ (mp-28933) + -6.1224 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 3.7449 Li ₂ O(mp-1960) + 0.5102 LiC ₁₂ (mp-1021323)	-2	0.897
6	0.323	0.5 Br ₂ O ₃ (mp-28933) + -4.6531 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 3.8061 Li ₂ O(mp-1960) + 0.3878 LiC ₁₂ (mp-1021323)	-1.535	0.897
5	1.117	1.0 C(mp-569304) + -1.0 CO ₂ (mp-20066) + 2.0 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280) + 3.0 LiCl(mp-1185319)	-0.284	0.896
5	1.127	-0.96 CO ₂ (mp-20066) + 1.96 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280) + 0.08 LiC ₁₂ (mp-1021323) + 3.0 LiCl(mp-1185319)	-0.288	0.895
6	0.462	1.5 Cl ₂ O ₇ (mp-31050) + 3.5 Li ₂ O(mp-1960) + 1.0 LiBr(mp-976280) + -6.0 O ₂ (mp-12957)	0.186	0.895
6	0.522	3.0 ClO ₃ (mp-22869) + 3.5 Li ₂ O(mp-1960) + 1.0 LiBr(mp-976280) + -5.25 O ₂ (mp-12957)	0.184	0.894
6	0.607	7.0 C(mp-569304) + -7.0 CO ₂ (mp-20066) + 2.0 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280) + 3.0 LiClO ₄ (mp-30301)	-1.824	0.892
6	0.7	0.5 Br ₂ O ₃ (mp-28933) + -2.16 CO ₂ (mp-20066) + 2.41 Li ₂ O ₂ (mp-841) + 0.18 LiC ₁₂ (mp-1021323) + 3.0 LiCl(mp-1185319)	-0.676	0.89
6	0.75	2.0 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280) + 3.0 LiClO ₄ (mp-30301) + -7.0 O ₂ (mp-12957)	0.585	0.888
6	0.9	-48.0 CO ₂ (mp-20066) + 1.0 LiBr(mp-976280) + 4.0 LiC ₁₂ (mp-1021323) + 3.0 LiCl(mp-1185319) + 49.0 O ₂ (mp-12957)	-17.383	0.884
6	0.912	6.0 C(mp-569304) + -8.0 CO ₂ (mp-20066) + 2.0 Li ₂ CO ₃ (mp-3054) + 1.0 LiBr(mp-976280) + 3.0 LiClO ₄ (mp-30301)	-1.178	0.883
6	0.919	-9.1327 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 3.2551 Li ₂ CO ₃ (mp-3054) + 1.0 LiBr(mp-976280) + 0.4898 LiC ₁₂ (mp-1021323)	-1.357	0.883
6	0.925	-8.4286 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 3.2857 Li ₂ CO ₃ (mp-3054) + 1.0 LiBr(mp-976280) + 0.4286 LiC ₁₂ (mp-1021323)	-1.089	0.883

6	1.08	-3.5 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 3.5 Li ₂ CO ₃ (mp-3054) + 1.0 LiBr(mp-976280) + -6.0 O ₂ (mp-12957)	0.815	0.876
6	1.12	-2.0 CO ₂ (mp-20066) + 2.0 Li ₂ CO ₃ (mp-3054) + 1.0 LiBr(mp-976280) + 3.0 LiClO ₄ (mp-30301) + -6.0 O ₂ (mp-12957)	0.887	0.875
7	0.311	0.5 Br ₂ O ₃ (mp-28933) + -6.8571 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 3.7143 Li ₂ O(mp-1960) + 0.5714 LiC ₁₂ (mp-1021323)	-2.263	0.874
7	0.314	0.5 Br ₂ O ₃ (mp-28933) + 6.25 C(mp-569304) + -6.25 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 4.0 Li ₂ O(mp-1960)	-1.934	0.874
7	0.476	0.5 Br ₂ O ₃ (mp-28933) + 3.0 ClO ₃ (mp-22869) + 4.0 Li ₂ O(mp-1960) + -6.25 O ₂ (mp-12957)	0.218	0.871
7	0.606	0.5 Br ₂ O ₃ (mp-28933) + -8.64 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 3.64 Li ₂ O ₂ (mp-841) + 0.72 LiC ₁₂ (mp-1021323)	-2.804	0.869
7	0.608	-7.44 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 3.19 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280) + 0.62 LiC ₁₂ (mp-1021323)	-2.417	0.869
7	0.61	-6.72 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 3.22 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280) + 0.56 LiC ₁₂ (mp-1021323)	-2.158	0.869
7	0.616	5.5 C(mp-569304) + -5.5 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 3.5 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280)	-1.676	0.869
7	0.617	-5.28 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 3.28 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280) + 0.44 LiC ₁₂ (mp-1021323)	-1.702	0.869
6	1.268	-3.5 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 3.5 Li ₂ CO ₃ (mp-3054) + 1.0 LiBr(mp-976280) + -3.75 O ₂ (mp-12957)	0.746	0.868
7	0.698	0.5 Br ₂ O ₃ (mp-28933) + 3.0 ClO ₃ (mp-22869) + 4.0 Li ₂ O ₂ (mp-841) + -8.25 O ₂ (mp-12957)	0.333	0.867
5	1.6	0.5 Br ₂ O ₃ (mp-28933) + -60.0 CO ₂ (mp-20066) + 5.0 LiC ₁₂ (mp-1021323) + 3.0 LiClO ₄ (mp-30301) + 54.25 O ₂ (mp-12957)	-21.171	0.867
7	0.707	1.5 Cl ₂ O ₇ (mp-31050) + 3.5 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280) + -7.75 O ₂ (mp-12957)	0.287	0.867
7	0.737	3.0 ClO ₃ (mp-22869) + 3.5 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280) + -7.0 O ₂ (mp-12957)	0.284	0.866
5	1.68	0.5 Br ₂ O ₃ (mp-28933) + -3.4388 CO ₂ (mp-20066) + 2.4592 Li ₂ CO ₃ (mp-3054) + 0.0816 LiC ₁₂ (mp-1021323) + 3.0 LiCl(mp-1185319)	0.125	0.862
7	0.926	5.25 C(mp-569304) + -8.75 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 3.5 Li ₂ CO ₃ (mp-3054) + 1.0 LiBr(mp-976280)	-0.994	0.861
7	0.947	3.75 C(mp-569304) + -7.25 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 3.5 Li ₂ CO ₃ (mp-3054) + 1.0 LiBr(mp-976280)	-0.545	0.86

7	1.131	-3.5 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 3.5 Li ₂ CO ₃ (mp-3054) + 1.0 LiBr(mp-976280) + -5.25 O ₂ (mp-12957)	0.813	0.853
8	0.304	0.5 Br ₂ O ₃ (mp-28933) + -6.8571 CO ₂ (mp-20066) + 2.2143 Li ₂ O(mp-1960) + 0.5714 LiC ₁₂ (mp-1021323) + 3.0 LiClO ₄ (mp-30301)	-1.921	0.851
7	1.2	0.5 Br ₂ O ₃ (mp-28933) + -60.0 CO ₂ (mp-20066) + 5.0 LiC ₁₂ (mp-1021323) + 3.0 LiCl(mp-1185319) + 60.25 O ₂ (mp-12957)	-21.695	0.85
4	2.042	0.5 Br ₂ O ₃ (mp-28933) + 2.5 Li ₂ O ₂ (mp-841) + 3.0 LiCl(mp-1185319) + -2.25 O ₂ (mp-12957)	0.109	0.849
5	1.878	0.5 Br ₂ O ₃ (mp-28933) + -2.5 CO ₂ (mp-20066) + 2.5 Li ₂ CO ₃ (mp-3054) + 3.0 LiClO ₄ (mp-30301) + -7.0 O ₂ (mp-12957)	1.012	0.848
8	0.592	0.5 Br ₂ O ₃ (mp-28933) + 3.0 ClO ₂ (mp-23207) + 4.0 Li ₂ O(mp-1960) + -4.75 O ₂ (mp-12957)	0.151	0.847
8	0.605	0.5 Br ₂ O ₃ (mp-28933) + 8.25 C(mp-569304) + -8.25 CO ₂ (mp-20066) + 2.5 Li ₂ O ₂ (mp-841) + 3.0 LiClO ₄ (mp-30301)	-2.206	0.847
8	0.605	0.5 Br ₂ O ₃ (mp-28933) + -7.92 CO ₂ (mp-20066) + 2.17 Li ₂ O ₂ (mp-841) + 0.66 LiC ₁₂ (mp-1021323) + 3.0 LiClO ₄ (mp-30301)	-2.244	0.847
8	0.607	0.5 Br ₂ O ₃ (mp-28933) + 8.25 C(mp-569304) + -8.25 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 4.0 Li ₂ O ₂ (mp-841)	-2.507	0.847
8	0.608	7.75 C(mp-569304) + -7.75 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 3.5 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280)	-2.381	0.847
8	0.61	7.0 C(mp-569304) + -7.0 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 3.5 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280)	-2.125	0.847
8	0.611	0.5 Br ₂ O ₃ (mp-28933) + -6.48 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 3.73 Li ₂ O ₂ (mp-841) + 0.54 LiC ₁₂ (mp-1021323)	-2.089	0.847
8	0.679	0.5 Br ₂ O ₃ (mp-28933) + 1.5 Cl ₂ O ₇ (mp-31050) + 4.0 Li ₂ O ₂ (mp-841) + -9.0 O ₂ (mp-12957)	0.336	0.845
8	0.698	0.5 Br ₂ O ₃ (mp-28933) + 2.25 C(mp-569304) + -2.25 CO ₂ (mp-20066) + 2.5 Li ₂ O ₂ (mp-841) + 3.0 LiCl(mp-1185319)	-0.665	0.845
8	0.819	3.0 ClO ₂ (mp-23207) + 3.5 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280) + -5.5 O ₂ (mp-12957)	0.217	0.842
8	0.9	-84.0 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 1.0 LiBr(mp-976280) + 7.0 LiC ₁₂ (mp-1021323) + 80.5 O ₂ (mp-12957)	-30.242	0.84
8	0.92	6.0 C(mp-569304) + -9.5 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 3.5 Li ₂ CO ₃ (mp-3054) + 1.0 LiBr(mp-976280)	-1.25	0.839
9	0.304	0.5 Br ₂ O ₃ (mp-28933) + 7.0 C(mp-569304) + -7.0 CO ₂ (mp-20066) + 2.5 Li ₂ O(mp-1960) + 3.0 LiClO ₄ (mp-30301)	-1.847	0.83

9	0.323	0.5 Br ₂ O ₃ (mp-28933) + 4.75 C(mp-569304) + -4.75 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 4.0 Li ₂ O(mp-1960)	-1.484	0.83
9	0.434	0.5 Br ₂ O ₃ (mp-28933) + 1.5 Cl ₂ O ₇ (mp-31050) + 4.0 Li ₂ O(mp-1960) + -7.0 O ₂ (mp-12957)	0.221	0.829
7	1.684	0.5 Br ₂ O ₃ (mp-28933) + 1.0 C(mp-569304) + -3.5 CO ₂ (mp-20066) + 2.5 Li ₂ CO ₃ (mp-3054) + 3.0 LiCl(mp-1185319)	0.143	0.827
8	1.617	0.5 Br ₂ O ₃ (mp-28933) + -9.0714 CO ₂ (mp-20066) + 2.2143 Li ₂ CO ₃ (mp-3054) + 0.5714 LiC ₁₂ (mp-1021323) + 3.0 LiClO ₄ (mp-30301)	-1.523	0.812
8	1.617	0.5 Br ₂ O ₃ (mp-28933) + 7.0 C(mp-569304) + -9.5 CO ₂ (mp-20066) + 2.5 Li ₂ CO ₃ (mp-3054) + 3.0 LiClO ₄ (mp-30301)	-1.398	0.812
10	0.606	0.5 Br ₂ O ₃ (mp-28933) + 9.0 C(mp-569304) + -9.0 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 4.0 Li ₂ O ₂ (mp-841)	-2.762	0.805
10	0.611	0.5 Br ₂ O ₃ (mp-28933) + 6.75 C(mp-569304) + -6.75 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 4.0 Li ₂ O ₂ (mp-841)	-2.058	0.805
10	0.9	-84.0 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 1.0 LiBr(mp-976280) + 7.0 LiC ₁₂ (mp-1021323) + 79.75 O ₂ (mp-12957)	-30.24	0.799
10	0.9	-84.0 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 1.0 LiBr(mp-976280) + 7.0 LiC ₁₂ (mp-1021323) + 82.0 O ₂ (mp-12957)	-30.31	0.799
11	0.311	0.5 Br ₂ O ₃ (mp-28933) + 7.0 C(mp-569304) + -7.0 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 4.0 Li ₂ O(mp-1960)	-2.189	0.791
11	0.745	0.5 Br ₂ O ₃ (mp-28933) + 3.0 ClO ₂ (mp-23207) + 4.0 Li ₂ O ₂ (mp-841) + -6.75 O ₂ (mp-12957)	0.266	0.783
7	2.96	0.5 Br ₂ O ₃ (mp-28933) + -9.8673 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 3.7449 Li ₂ CO ₃ (mp-3054) + 0.5102 LiC ₁₂ (mp-1021323)	-1.326	0.747
7	2.964	0.5 Br ₂ O ₃ (mp-28933) + 6.25 C(mp-569304) + -10.25 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 4.0 Li ₂ CO ₃ (mp-3054)	-1.214	0.746
8	2.948	0.5 Br ₂ O ₃ (mp-28933) + -10.5714 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 3.7143 Li ₂ CO ₃ (mp-3054) + 0.5714 LiC ₁₂ (mp-1021323)	-1.595	0.734
8	2.998	0.5 Br ₂ O ₃ (mp-28933) + -8.4592 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 3.8061 Li ₂ CO ₃ (mp-3054) + 0.3878 LiC ₁₂ (mp-1021323)	-0.85	0.731
8	3.006	0.5 Br ₂ O ₃ (mp-28933) + 4.75 C(mp-569304) + -8.75 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 4.0 Li ₂ CO ₃ (mp-3054)	-0.765	0.73
7	3.393	0.5 Br ₂ O ₃ (mp-28933) + -4.0 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 4.0 Li ₂ CO ₃ (mp-3054) + -7.0 O ₂ (mp-12957)	0.94	0.716

6	3.646	0.5 Br ₂ O ₃ (mp-28933) + -2.5 CO ₂ (mp-20066) + 2.5 Li ₂ CO ₃ (mp-3054) + 3.0 LiCl(mp-1185319) + -1.0 O ₂ (mp-12957)	0.487	0.708
9	3.511	0.5 Br ₂ O ₃ (mp-28933) + -4.0 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 4.0 Li ₂ CO ₃ (mp-3054) + -6.25 O ₂ (mp-12957)	0.937	0.683
12	2.952	0.5 Br ₂ O ₃ (mp-28933) + 7.0 C(mp-569304) + -11.0 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 4.0 Li ₂ CO ₃ (mp-3054)	-1.47	0.677
10	3.798	0.5 Br ₂ O ₃ (mp-28933) + -4.0 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 4.0 Li ₂ CO ₃ (mp-3054) + -4.75 O ₂ (mp-12957)	0.87	0.651
4	4.7	0.5 Br ₂ O ₃ (mp-28933) + 2.5 Li ₂ O(mp-1960) + 3.0 LiCl(mp-1185319) + -1.0 O ₂ (mp-12957)	0.037	0.642
9	7.302	0.5 Br ₂ O ₃ (mp-28933) + -96.0 CO ₂ (mp-20066) + 1.5 Cl ₂ O ₇ (mp-31050) + 8.0 LiC ₁₂ (mp-1021323) + 91.0 O ₂ (mp-12957)	-34.552	0.401
12	7.302	0.5 Br ₂ O ₃ (mp-28933) + -96.0 CO ₂ (mp-20066) + 3.0 ClO ₃ (mp-22869) + 8.0 LiC ₁₂ (mp-1021323) + 91.75 O ₂ (mp-12957)	-34.555	0.379
13	7.302	0.5 Br ₂ O ₃ (mp-28933) + -96.0 CO ₂ (mp-20066) + 3.0 ClO ₂ (mp-23207) + 8.0 LiC ₁₂ (mp-1021323) + 93.25 O ₂ (mp-12957)	-34.622	0.374
4	9.313	2.0 Li ₂ O ₂ (mp-841) + 1.0 LiBr(mp-976280) + 3.0 LiCl(mp-1185319) + -1.0 O ₂ (mp-12957)	0.061	0.315
2	12.062	-2.0 CO ₂ (mp-20066) + 2.0 Li ₂ CO ₃ (mp-3054) + 1.0 LiBr(mp-976280) + 3.0 LiCl(mp-1185319)	0.363	0.244

Table S6. List of candidate solid state reactions for $I4/mmm$ $\text{Li}_7\text{O}_2\text{FBr}_2$ inverse-perovskite compound based on a data-driven approach in Reference 76 of the main text. Reactions are summarized with their number of competing phases that formed aside from the target phase, nucleation barrier based on classical nucleation theory, reaction enthalpy, and multi-objective decision-making metric called TOPSIS score. Compound tags in parenthesis indicate the Materials Project ID.

Number of competing phases	Nucleation barrier / a.u.	Reaction summary	Enthalpy / eV	TOPSIS score
2	0.843	1.0 C(mp-569304) + -1.0 CO ₂ (mp-20066) + 2.0 Li ₂ O ₂ (mp-841) + 2.0 LiBr(mp-976280) + 1.0 LiF(mp-1138)	-0.26	0.917
2	0.848	-0.96 CO ₂ (mp-20066) + 1.96 Li ₂ O ₂ (mp-841) + 2.0 LiBr(mp-976280) + 0.08 LiC ₁₂ (mp-1021323) + 1.0 LiF(mp-1138)	-0.265	0.917
4	0.838	1.0 Br ₂ O ₃ (mp-28933) + 3.0 Li ₂ O(mp-1960) + 1.0 LiF(mp-1138) + -2.0 O ₂ (mp-12957)	0.155	0.791
4	0.87	1.0 Br ₂ O ₃ (mp-28933) + 3.0 Li ₂ O ₂ (mp-841) + 1.0 LiF(mp-1138) + -3.5 O ₂ (mp-12957)	0.256	0.79
4	0.9	-48.0 CO ₂ (mp-20066) + 2.0 LiBr(mp-976280) + 4.0 LiC ₁₂ (mp-1021323) + 1.0 LiF(mp-1138) + 49.0 O ₂ (mp-12957)	-20.21	0.79
5	0.329	1.0 Br ₂ O ₃ (mp-28933) + -1.9592 CO ₂ (mp-20066) + 2.9184 Li ₂ O(mp-1960) + 0.1633 LiC ₁₂ (mp-1021323) + 1.0 LiF(mp-1138)	-0.673	0.746
5	0.33	1.0 Br ₂ O ₃ (mp-28933) + 2.0 C(mp-569304) + -2.0 CO ₂ (mp-20066) + 3.0 Li ₂ O(mp-1960) + 1.0 LiF(mp-1138)	-0.648	0.746
5	0.616	1.0 Br ₂ O ₃ (mp-28933) + 3.5 C(mp-569304) + -3.5 CO ₂ (mp-20066) + 3.0 Li ₂ O ₂ (mp-841) + 1.0 LiF(mp-1138)	-1.15	0.742
5	0.616	1.0 Br ₂ O ₃ (mp-28933) + -3.36 CO ₂ (mp-20066) + 2.86 Li ₂ O ₂ (mp-841) + 0.28 LiC ₁₂ (mp-1021323) + 1.0 LiF(mp-1138)	-1.169	0.742
5	2.9	1.0 Br ₂ O ₃ (mp-28933) + -72.0 CO ₂ (mp-20066) + 6.0 LiC ₁₂ (mp-1021323) + 1.0 LiF(mp-1138) + 71.5 O ₂ (mp-12957)	-30.271	0.69
5	3.127	1.0 Br ₂ O ₃ (mp-28933) + -4.8776 CO ₂ (mp-20066) + 2.9184 Li ₂ CO ₃ (mp-3054) + 0.1633 LiC ₁₂ (mp-1021323) + 1.0 LiF(mp-1138)	-0.061	0.683
5	3.129	1.0 Br ₂ O ₃ (mp-28933) + 2.0 C(mp-569304) + -5.0 CO ₂ (mp-20066) + 3.0 Li ₂ CO ₃ (mp-3054) + 1.0 LiF(mp-1138)	-0.019	0.683
4	4.678	1.0 Br ₂ O ₃ (mp-28933) + -3.0 CO ₂ (mp-20066) + 3.0 Li ₂ CO ₃ (mp-3054) + 1.0 LiF(mp-1138) + -2.0 O ₂ (mp-12957)	0.784	0.663
2	12.039	2.0 Li ₂ O ₂ (mp-841) + 2.0 LiBr(mp-976280) + 1.0 LiF(mp-1138) + -1.0 O ₂ (mp-12957)	0.142	0.334
1	16.307	-2.0 CO ₂ (mp-20066) + 2.0 Li ₂ CO ₃ (mp-3054) + 2.0 LiBr(mp-976280) + 1.0 LiF(mp-1138)	0.494	0.254

Table S7. List of candidate solid state reactions for $Fm\bar{3}m$ Li_6OSeI_2 inverse-perovskite compound based on a data-driven approach in Reference 76 of the main text. Reactions are summarized with their number of competing phases that formed aside from the target phase, nucleation barrier based on classical nucleation theory, reaction enthalpy, and multi-objective decision-making metric called TOPSIS score. Compound tags in parenthesis indicate the Materials Project ID.

Number of competing phases	Nucleation barrier / a.u.	Reaction summary	Enthalpy / eV	TOPSIS score
0	0.119	-3.8163 $\text{CO}_2(\text{mp-20066}) + 0.8776 \text{Li}_2\text{CO}_3(\text{mp-3054}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286}) + 0.2449 \text{LiC12}(\text{mp-1021323}) + 2.0 \text{LiIO}_3(\text{mp-23384})$	-0.308	1
0	0.12	3.0 $\text{C}(\text{mp-569304}) + -4.0 \text{CO}_2(\text{mp-20066}) + 1.0 \text{Li}_2\text{CO}_3(\text{mp-3054}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286}) + 2.0 \text{LiIO}_3(\text{mp-23384})$	-0.233	1
0	0.121	-2.9388 $\text{CO}_2(\text{mp-20066}) + 0.8776 \text{Li}_2\text{O}(\text{mp-1960}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286}) + 0.2449 \text{LiC12}(\text{mp-1021323}) + 2.0 \text{LiIO}_3(\text{mp-23384})$	-0.529	1
0	0.122	3.0 $\text{C}(\text{mp-569304}) + -3.0 \text{CO}_2(\text{mp-20066}) + 1.0 \text{Li}_2\text{O}(\text{mp-1960}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286}) + 2.0 \text{LiIO}_3(\text{mp-23384})$	-0.485	1
0	0.154	1.5 $\text{C}(\text{mp-569304}) + -1.5 \text{CO}_2(\text{mp-20066}) + 2.0 \text{I}(\text{mp-23153}) + 2.0 \text{Li}_2\text{O}_2(\text{mp-841}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286})$	-0.456	0.999
0	0.155	-1.44 $\text{CO}_2(\text{mp-20066}) + 2.0 \text{I}(\text{mp-23153}) + 1.94 \text{Li}_2\text{O}_2(\text{mp-841}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286}) + 0.12 \text{LiC12}(\text{mp-1021323})$	-0.466	0.999
0	0.39	-2.4694 $\text{CO}_2(\text{mp-20066}) + 2.0 \text{I}(\text{mp-23153}) + 1.9796 \text{Li}_2\text{CO}_3(\text{mp-3054}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286}) + 0.0408 \text{LiC12}(\text{mp-1021323})$	0.436	0.994
0	0.393	0.5 $\text{C}(\text{mp-569304}) + -2.5 \text{CO}_2(\text{mp-20066}) + 2.0 \text{I}(\text{mp-23153}) + 2.0 \text{Li}_2\text{CO}_3(\text{mp-3054}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286})$	0.449	0.994
0	0.616	0.5 $\text{C}(\text{mp-569304}) + -0.5 \text{CO}_2(\text{mp-20066}) + 1.0 \text{Li}_2\text{O}_2(\text{mp-841}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286}) + 2.0 \text{LiI}(\text{mp-570935})$	-0.141	0.99
0	0.629	-0.48 $\text{CO}_2(\text{mp-20066}) + 0.98 \text{Li}_2\text{O}_2(\text{mp-841}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286}) + 0.04 \text{LiC12}(\text{mp-1021323}) + 2.0 \text{LiI}(\text{mp-570935})$	-0.145	0.99
0	1.05	-0.4898 $\text{CO}_2(\text{mp-20066}) + 2.0 \text{I}(\text{mp-23153}) + 1.9796 \text{Li}_2\text{O}(\text{mp-1960}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286}) + 0.0408 \text{LiC12}(\text{mp-1021323})$	-0.062	0.982
0	1.083	0.5 $\text{C}(\text{mp-569304}) + -0.5 \text{CO}_2(\text{mp-20066}) + 2.0 \text{I}(\text{mp-23153}) + 2.0 \text{Li}_2\text{O}(\text{mp-1960}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286})$	-0.055	0.981
1	0.114	3.5 $\text{C}(\text{mp-569304}) + -3.5 \text{CO}_2(\text{mp-20066}) + 1.0 \text{Li}_2\text{O}_2(\text{mp-841}) + 1.0 \text{Li}_2\text{Se}(\text{mp-2286}) + 2.0 \text{LiIO}_3(\text{mp-23384})$	-0.685	0.97

1	0.115	-3.36 CO ₂ (mp-20066) + 0.86 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 0.28 LiC ₁₂ (mp-1021323) + 2.0 LiIO ₃ (mp-23384)	-0.708	0.97
4	0.116	-2.9388 CO ₂ (mp-20066) + 1.0 I ₂ O ₅ (mp-23261) + 1.8776 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 0.2449 LiC ₁₂ (mp-1021323)	-0.767	0.886
4	0.116	3.0 C(mp-569304) + -3.0 CO ₂ (mp-20066) + 1.0 I ₂ O ₅ (mp-23261) + 2.0 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286)	-0.723	0.886
5	0.113	-4.8163 CO ₂ (mp-20066) + 1.0 I ₂ O ₅ (mp-23261) + 1.8776 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 0.2449 LiC ₁₂ (mp-1021323)	-0.294	0.859
5	0.113	3.0 C(mp-569304) + -5.0 CO ₂ (mp-20066) + 1.0 I ₂ O ₅ (mp-23261) + 2.0 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286)	-0.219	0.859
6	0.108	4.0 C(mp-569304) + -4.0 CO ₂ (mp-20066) + 1.0 I ₂ O ₅ (mp-23261) + 2.0 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286)	-1.124	0.834
6	0.108	-3.84 CO ₂ (mp-20066) + 1.0 I ₂ O ₅ (mp-23261) + 1.84 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 0.32 LiC ₁₂ (mp-1021323)	-1.15	0.834
7	0.1	-24.0 CO ₂ (mp-20066) + 1.0 Li ₂ Se(mp-2286) + 2.0 LiC ₁₂ (mp-1021323) + 2.0 LiI(mp-570935) + 24.5 O ₂ (mp-12957)	-12.111	0.81
7	0.1	-24.0 CO ₂ (mp-20066) + 1.0 Li ₂ Se(mp-2286) + 2.0 LiC ₁₂ (mp-1021323) + 2.0 LiIO ₃ (mp-23384) + 21.5 O ₂ (mp-12957)	-11.209	0.81
11	2.837	-2.0 CO ₂ (mp-20066) + 2.0 I(mp-23153) + 2.0 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + -0.5 O ₂ (mp-12957)	0.69	0.71
11	3.029	2.0 I(mp-23153) + 2.0 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + -1.5 O ₂ (mp-12957)	0.267	0.709
13	0.1	-48.0 CO ₂ (mp-20066) + 1.0 I ₂ O ₅ (mp-23261) + 1.0 Li ₂ Se(mp-2286) + 4.0 LiC ₁₂ (mp-1021323) + 46.0 O ₂ (mp-12957)	-23.618	0.688
13	0.858	1.0 I ₂ O ₅ (mp-23261) + 2.0 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + -4.0 O ₂ (mp-12957)	0.804	0.684
14	0.832	-2.0 CO ₂ (mp-20066) + 1.0 I ₂ O ₅ (mp-23261) + 2.0 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + -3.0 O ₂ (mp-12957)	1.227	0.668
11	9.322	1.0 I ₂ O ₅ (mp-23261) + 2.0 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + -3.0 O ₂ (mp-12957)	0.723	0.653
16	0.1	-48.0 CO ₂ (mp-20066) + 2.0 I(mp-23153) + 1.0 Li ₂ Se(mp-2286) + 4.0 LiC ₁₂ (mp-1021323) + 48.5 O ₂ (mp-12957)	-24.155	0.641
0	40.268	-1.0 CO ₂ (mp-20066) + 1.0 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 2.0 LiI(mp-570935)	0.311	0.396
9	45.946	1.0 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 2.0 LiI(mp-570935) + -0.5 O ₂ (mp-12957)	0.1	0.19

Table S8. List of candidate solid state reactions for *Cmcm* Li₁₂O₃SeClBr₃ inverse-perovskite compound based on a data-driven approach in Reference 76 of the main text. Reactions are summarized with their number of competing phases that formed aside from the target phase, nucleation barrier based on classical nucleation theory, reaction enthalpy, and multi-objective decision-making metric called TOPSIS score. Compound tags in parenthesis indicate the Materials Project ID.

Number of competing phases	Nucleation barrier / a.u.	Reaction summary	Enthalpy / eV	TOPSIS score
3	0.105	1.5 Br ₂ O ₃ (mp-28933) + -6.96 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 4.71 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 0.58 LiC ₁₂ (mp-1021323)	-1.457	1
3	0.195	-1.9592 CO ₂ (mp-20066) + 2.9184 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.1633 LiC ₁₂ (mp-1021323) + 1.0 LiClO ₄ (mp-30301)	-0.275	0.996
4	0.163	-4.8776 CO ₂ (mp-20066) + 2.9184 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.1633 LiC ₁₂ (mp-1021323) + 1.0 LiClO ₄ (mp-30301)	0.092	0.979
4	0.197	2.0 C(mp-569304) + -2.0 CO ₂ (mp-20066) + 3.0 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 1.0 LiClO ₄ (mp-30301)	-0.261	0.979
5	0.121	1.5 Br ₂ O ₃ (mp-28933) + -7.3163 CO ₂ (mp-20066) + 4.3776 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 0.2449 LiC ₁₂ (mp-1021323) + 1.0 LiCl(mp-1185319)	-0.023	0.959
5	0.127	-3.36 CO ₂ (mp-20066) + 2.86 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.28 LiC ₁₂ (mp-1021323) + 1.0 LiClO ₄ (mp-30301)	-0.573	0.959
5	0.131	1.5 Br ₂ O ₃ (mp-28933) + -2.9388 CO ₂ (mp-20066) + 4.3776 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 0.2449 LiC ₁₂ (mp-1021323) + 1.0 LiCl(mp-1185319)	-0.574	0.959
5	0.131	1.5 Br ₂ O ₃ (mp-28933) + 3.0 C(mp-569304) + -3.0 CO ₂ (mp-20066) + 4.5 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 1.0 LiCl(mp-1185319)	-0.552	0.959
5	0.203	-1.7143 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 3.4286 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.1429 LiC ₁₂ (mp-1021323)	-0.294	0.959
5	0.205	1.75 C(mp-569304) + -1.75 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 3.5 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280)	-0.281	0.959
5	0.214	-4.6735 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 3.449 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.102 LiC ₁₂ (mp-1021323)	0.249	0.959

5	0.268	1.5 C(mp-569304) + -1.5 CO2(mp-20066) + 3.0 Li2O2(mp-841) + 1.0 Li2Se(mp-2286) + 3.0 LiBr(mp-976280) + 1.0 LiCl(mp-1185319)	-0.202	0.958
5	0.272	-1.44 CO2(mp-20066) + 2.94 Li2O2(mp-841) + 1.0 Li2Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.12 LiC12(mp-1021323) + 1.0 LiCl(mp-1185319)	-0.207	0.958
5	0.327	-1.2245 CO2(mp-20066) + 1.0 ClO2(mp-23207) + 3.449 Li2O(mp-1960) + 1.0 Li2Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.102 LiC12(mp-1021323)	-0.185	0.958
5	0.332	1.25 C(mp-569304) + -1.25 CO2(mp-20066) + 1.0 ClO2(mp-23207) + 3.5 Li2O(mp-1960) + 1.0 Li2Se(mp-2286) + 3.0 LiBr(mp-976280)	-0.176	0.958
6	0.1	1.5 Br2O3(mp-28933) + -108.0 CO2(mp-20066) + 1.0 Li2Se(mp-2286) + 9.0 LiC12(mp-1021323) + 1.0 LiClO4(mp-30301) + 105.25 O2(mp-12957)	-27.09	0.94
6	0.11	1.5 Br2O3(mp-28933) + -5.04 CO2(mp-20066) + 4.29 Li2O2(mp-841) + 1.0 Li2Se(mp-2286) + 0.42 LiC12(mp-1021323) + 1.0 LiCl(mp-1185319)	-1.02	0.94
6	0.111	1.5 Br2O3(mp-28933) + -4.6531 CO2(mp-20066) + 1.0 ClO3(mp-22869) + 4.8061 Li2O(mp-1960) + 1.0 Li2Se(mp-2286) + 0.3878 LiC12(mp-1021323)	-0.967	0.94
6	0.114	1.5 Br2O3(mp-28933) + -4.1633 CO2(mp-20066) + 1.0 ClO2(mp-23207) + 4.8265 Li2O(mp-1960) + 1.0 Li2Se(mp-2286) + 0.3469 LiC12(mp-1021323)	-0.858	0.94
6	0.126	3.5 C(mp-569304) + -3.5 CO2(mp-20066) + 3.0 Li2O2(mp-841) + 1.0 Li2Se(mp-2286) + 3.0 LiBr(mp-976280) + 1.0 LiClO4(mp-30301)	-0.562	0.94
6	0.149	-5.3776 CO2(mp-20066) + 0.5 Cl2O7(mp-31050) + 3.4184 Li2CO3(mp-3054) + 1.0 Li2Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.1633 LiC12(mp-1021323)	0.075	0.94
6	0.163	-5.1429 CO2(mp-20066) + 1.0 ClO3(mp-22869) + 3.4286 Li2CO3(mp-3054) + 1.0 Li2Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.1429 LiC12(mp-1021323)	0.138	0.939
6	0.164	2.0 C(mp-569304) + -5.0 CO2(mp-20066) + 3.0 Li2CO3(mp-3054) + 1.0 Li2Se(mp-2286) + 3.0 LiBr(mp-976280) + 1.0 LiClO4(mp-30301)	0.117	0.939
6	0.174	-1.9592 CO2(mp-20066) + 0.5 Cl2O7(mp-31050) + 3.4184 Li2O(mp-1960) + 1.0 Li2Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.1633 LiC12(mp-1021323)	-0.355	0.939
6	0.176	2.0 C(mp-569304) + -2.0 CO2(mp-20066) + 0.5 Cl2O7(mp-31050) + 3.5 Li2O(mp-1960) + 1.0 Li2Se(mp-2286) + 3.0 LiBr(mp-976280)	-0.34	0.939

6	0.205	1.5 Br ₂ O ₃ (mp-28933) + -4.5 CO ₂ (mp-20066) + 4.5 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 1.0 LiClO ₄ (mp-30301) + -5.0 O ₂ (mp-12957)	0.86	0.939
7	0.1	1.5 Br ₂ O ₃ (mp-28933) + -108.0 CO ₂ (mp-20066) + 1.0 Li ₂ Se(mp-2286) + 9.0 LiC ₁₂ (mp-1021323) + 1.0 LiCl(mp-1185319) + 107.25 O ₂ (mp-12957)	-27.212	0.921
7	0.105	1.5 Br ₂ O ₃ (mp-28933) + -7.2 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 4.7 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 0.6 LiC ₁₂ (mp-1021323)	-1.517	0.921
7	0.109	1.5 Br ₂ O ₃ (mp-28933) + -9.4592 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 4.8061 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 0.3878 LiC ₁₂ (mp-1021323)	-0.362	0.921
7	0.109	1.5 Br ₂ O ₃ (mp-28933) + 4.75 C(mp-569304) + -9.75 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 5.0 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286)	-0.302	0.921
7	0.11	1.5 Br ₂ O ₃ (mp-28933) + -4.898 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 4.7959 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 0.4082 LiC ₁₂ (mp-1021323)	-1.028	0.921
7	0.112	1.5 Br ₂ O ₃ (mp-28933) + 4.75 C(mp-569304) + -4.75 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 5.0 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286)	-0.931	0.921
7	0.12	-3.6 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 3.35 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.3 LiC ₁₂ (mp-1021323)	-0.704	0.921
7	0.122	1.5 Br ₂ O ₃ (mp-28933) + 3.0 C(mp-569304) + -7.5 CO ₂ (mp-20066) + 4.5 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 1.0 LiCl(mp-1185319)	0.014	0.921
7	0.124	-3.36 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 3.36 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.28 LiC ₁₂ (mp-1021323)	-0.643	0.921
7	0.133	3.0 C(mp-569304) + -3.0 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 3.5 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280)	-0.527	0.921
7	0.133	-2.88 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 3.38 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 0.24 LiC ₁₂ (mp-1021323)	-0.537	0.921
7	0.164	1.75 C(mp-569304) + -5.25 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 3.5 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280)	0.16	0.921
7	0.176	1.5 Br ₂ O ₃ (mp-28933) + -5.0 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 5.0 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + -5.0 O ₂ (mp-12957)	0.843	0.921
7	0.215	1.25 C(mp-569304) + -4.75 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 3.5 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280)	0.264	0.92
7	0.284	1.5 Br ₂ O ₃ (mp-28933) + -4.5 CO ₂ (mp-20066) + 4.5 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 1.0 LiCl(mp-1185319) + -3.0 O ₂ (mp-12957)	0.737	0.92

8	0.1	1.5 Br ₂ O ₃ (mp-28933) + -120.0 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 1.0 Li ₂ Se(mp-2286) + 10.0 LiC ₁₂ (mp-1021323) + 117.5 O ₂ (mp-12957)	-30.212	0.903
8	0.1	1.5 Br ₂ O ₃ (mp-28933) + -120.0 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 1.0 Li ₂ Se(mp-2286) + 10.0 LiC ₁₂ (mp-1021323) + 118.25 O ₂ (mp-12957)	-30.229	0.903
8	0.105	1.5 Br ₂ O ₃ (mp-28933) + 7.25 C(mp-569304) + -7.25 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 5.0 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286)	-1.433	0.903
8	0.105	1.5 Br ₂ O ₃ (mp-28933) + 7.25 C(mp-569304) + -7.25 CO ₂ (mp-20066) + 4.5 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 1.0 LiClO ₄ (mp-30301)	-1.363	0.903
8	0.105	1.5 Br ₂ O ₃ (mp-28933) + -6.96 CO ₂ (mp-20066) + 4.21 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 0.58 LiC ₁₂ (mp-1021323) + 1.0 LiClO ₄ (mp-30301)	-1.386	0.903
8	0.106	1.5 Br ₂ O ₃ (mp-28933) + -6.48 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 4.73 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 0.54 LiC ₁₂ (mp-1021323)	-1.35	0.903
8	0.108	1.5 Br ₂ O ₃ (mp-28933) + -9.6939 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 4.7959 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 0.4082 LiC ₁₂ (mp-1021323)	-0.424	0.903
8	0.109	1.5 Br ₂ O ₃ (mp-28933) + -9.1939 CO ₂ (mp-20066) + 4.2959 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 0.4082 LiC ₁₂ (mp-1021323) + 1.0 LiClO ₄ (mp-30301)	-0.408	0.903
8	0.109	1.5 Br ₂ O ₃ (mp-28933) + 5.0 C(mp-569304) + -9.5 CO ₂ (mp-20066) + 4.5 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 1.0 LiClO ₄ (mp-30301)	-0.345	0.903
8	0.11	1.5 Br ₂ O ₃ (mp-28933) + 5.25 C(mp-569304) + -5.25 CO ₂ (mp-20066) + 4.5 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 1.0 LiCl(mp-1185319)	-1.003	0.903
8	0.111	1.5 Br ₂ O ₃ (mp-28933) + -8.9898 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 4.8265 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 0.3469 LiC ₁₂ (mp-1021323)	-0.251	0.903
8	0.111	1.5 Br ₂ O ₃ (mp-28933) + 4.25 C(mp-569304) + -9.25 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 5.0 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286)	-0.197	0.903
8	0.111	1.5 Br ₂ O ₃ (mp-28933) + -4.898 CO ₂ (mp-20066) + 4.2959 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 0.4082 LiC ₁₂ (mp-1021323) + 1.0 LiClO ₄ (mp-30301)	-0.948	0.903
8	0.12	3.75 C(mp-569304) + -3.75 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 3.5 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280)	-0.692	0.903

8	0.123	3.5 C(mp-569304) + -3.5 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 3.5 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280)	-0.632	0.903
8	0.149	2.0 C(mp-569304) + -5.5 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 3.5 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280)	0.1	0.903
8	0.288	1.5 Br ₂ O ₃ (mp-28933) + 4.5 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 1.0 LiCl(mp-1185319) + -5.25 O ₂ (mp-12957)	0.262	0.902
8	0.365	1.5 Br ₂ O ₃ (mp-28933) + 1.0 ClO ₂ (mp-23207) + 5.0 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + -4.25 O ₂ (mp-12957)	0.198	0.901
9	0.1	-72.0 CO ₂ (mp-20066) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 6.0 LiC ₁₂ (mp-1021323) + 1.0 LiClO ₄ (mp-30301) + 71.5 O ₂ (mp-12957)	-18.034	0.885
9	0.111	1.5 Br ₂ O ₃ (mp-28933) + 5.0 C(mp-569304) + -5.0 CO ₂ (mp-20066) + 4.5 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 1.0 LiClO ₄ (mp-30301)	-0.911	0.885
9	0.115	1.5 Br ₂ O ₃ (mp-28933) + 4.25 C(mp-569304) + -4.25 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 5.0 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286)	-0.827	0.885
9	0.79	1.5 Br ₂ O ₃ (mp-28933) + 4.5 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 1.0 LiCl(mp-1185319) + -3.0 O ₂ (mp-12957)	0.171	0.879
10	0.1	-72.0 CO ₂ (mp-20066) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 6.0 LiC ₁₂ (mp-1021323) + 1.0 LiCl(mp-1185319) + 73.5 O ₂ (mp-12957)	-18.157	0.868
10	0.105	1.5 Br ₂ O ₃ (mp-28933) + 7.5 C(mp-569304) + -7.5 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 5.0 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286)	-1.493	0.868
10	0.106	1.5 Br ₂ O ₃ (mp-28933) + 6.75 C(mp-569304) + -6.75 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 5.0 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286)	-1.328	0.868
10	0.183	1.5 Br ₂ O ₃ (mp-28933) + -5.0 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 5.0 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + -4.75 O ₂ (mp-12957)	0.842	0.868
10	0.198	1.5 Br ₂ O ₃ (mp-28933) + -5.0 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 5.0 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + -4.25 O ₂ (mp-12957)	0.827	0.868
10	0.207	1.5 Br ₂ O ₃ (mp-28933) + 4.5 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 1.0 LiClO ₄ (mp-30301) + -7.25 O ₂ (mp-12957)	0.384	0.868
10	0.36	1.5 Br ₂ O ₃ (mp-28933) + 4.5 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 1.0 LiClO ₄ (mp-30301) + -5.0 O ₂ (mp-12957)	0.294	0.867
11	0.1	1.5 Br ₂ O ₃ (mp-28933) + -120.0 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 1.0 Li ₂ Se(mp-2286) + 10.0 LiC ₁₂ (mp-1021323) + 117.75 O ₂ (mp-12957)	-30.213	0.852

11	0.11	1.5 Br ₂ O ₃ (mp-28933) + 5.0 C(mp-569304) + -5.0 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 5.0 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286)	-0.991	0.852
11	0.935	-3.5 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 3.5 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + -1.25 O ₂ (mp-12957)	0.566	0.844
12	0.108	1.5 Br ₂ O ₃ (mp-28933) + 5.0 C(mp-569304) + -10.0 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 5.0 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286)	-0.362	0.837
12	0.2	1.5 Br ₂ O ₃ (mp-28933) + 1.0 ClO ₂ (mp-23207) + 5.0 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + -6.75 O ₂ (mp-12957)	0.298	0.836
12	0.305	1.5 Br ₂ O ₃ (mp-28933) + 1.0 ClO ₃ (mp-22869) + 5.0 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + -4.75 O ₂ (mp-12957)	0.213	0.835
12	0.524	-3.5 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 3.5 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + -2.0 O ₂ (mp-12957)	0.582	0.833
12	1.124	-3.0 CO ₂ (mp-20066) + 3.0 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 1.0 LiClO ₄ (mp-30301) + -2.0 O ₂ (mp-12957)	0.599	0.826
12	1.162	3.0 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 1.0 LiClO ₄ (mp-30301) + -3.5 O ₂ (mp-12957)	0.282	0.826
13	0.1	-84.0 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 7.0 LiC ₁₂ (mp-1021323) + 84.0 O ₂ (mp-12957)	-21.157	0.822
13	0.185	1.5 Br ₂ O ₃ (mp-28933) + 1.0 ClO ₃ (mp-22869) + 5.0 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + -7.25 O ₂ (mp-12957)	0.314	0.821
13	0.536	0.5 Cl ₂ O ₇ (mp-31050) + 3.5 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + -3.75 O ₂ (mp-12957)	0.212	0.818
13	0.639	-3.5 CO ₂ (mp-20066) + 1.0 ClO ₃ (mp-22869) + 3.5 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + -1.75 O ₂ (mp-12957)	0.581	0.817
13	0.656	1.0 ClO ₃ (mp-22869) + 3.5 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + -3.5 O ₂ (mp-12957)	0.211	0.817
11	2.416	0.5 Cl ₂ O ₇ (mp-31050) + 3.5 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + -2.0 O ₂ (mp-12957)	0.142	0.816
14	0.1	-84.0 CO ₂ (mp-20066) + 0.5 Cl ₂ O ₇ (mp-31050) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 7.0 LiC ₁₂ (mp-1021323) + 83.75 O ₂ (mp-12957)	-21.157	0.807
14	0.1	-84.0 CO ₂ (mp-20066) + 1.0 ClO ₂ (mp-23207) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 7.0 LiC ₁₂ (mp-1021323) + 84.5 O ₂ (mp-12957)	-21.173	0.807

14	0.177	1.5 Br ₂ O ₃ (mp-28933) + 0.5 Cl ₂ O ₇ (mp-31050) + 5.0 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + -7.5 O ₂ (mp-12957)	0.315	0.807
14	0.276	1.5 Br ₂ O ₃ (mp-28933) + 0.5 Cl ₂ O ₇ (mp-31050) + 5.0 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + -5.0 O ₂ (mp-12957)	0.214	0.806
14	0.969	1.0 ClO ₂ (mp-23207) + 3.5 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + -3.0 O ₂ (mp-12957)	0.196	0.799
11	4.357	1.0 ClO ₃ (mp-22869) + 3.5 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + -1.75 O ₂ (mp-12957)	0.141	0.758
4	18.934	-3.0 CO ₂ (mp-20066) + 3.0 Li ₂ CO ₃ (mp-3054) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 1.0 LiCl(mp-1185319)	0.476	0.237
10	18.064	3.0 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 1.0 LiClO ₄ (mp-30301) + -2.0 O ₂ (mp-12957)	0.221	0.202
9	21.479	1.0 ClO ₂ (mp-23207) + 3.5 Li ₂ O(mp-1960) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + -1.25 O ₂ (mp-12957)	0.125	0.105
10	22.28	3.0 Li ₂ O ₂ (mp-841) + 1.0 Li ₂ Se(mp-2286) + 3.0 LiBr(mp-976280) + 1.0 LiCl(mp-1185319) + -1.5 O ₂ (mp-12957)	0.159	0.079