

## Supporting Information

### Discovery of Lead-Free Hybrid Organic/Inorganic Perovskites Using Metaheuristic-Driven DFT Calculations

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## List of contents

### **Supporting Discussion 1** Evidence supporting the apparent-structure-type concept

### **Supporting Discussion 2** Symmetry setting for band structure

**Figure S1.** The 27 different molecular arrangements for both  $(\text{NH}_3\text{OH})\text{PbCl}_3$  and  $(\text{CH}_3\text{NH}_3)\text{Cl}$  before the DFT-based structure relaxation, and their resultant orientations after the structure relaxation. The randomly located ‘A’-site molecule reorients during the DFT-based structure relaxation. The 27 random initial orientations achieved their final relaxed structures for both  $(\text{NH}_3\text{OH})\text{PbCl}_3$  and  $(\text{CH}_3\text{NH}_3)\text{Cl}$ .

**Figure S2.** Input model structures and their DFT-relaxed structures (from the 1<sup>st</sup> to 5<sup>th</sup> generations) used for NSGA-II.

**Figure S3.** Input model structures and the DFT-relaxed structures (from the 1<sup>st</sup> to 5<sup>th</sup> generations) used for NSGA-III.

**Figure S4.** The band structures (E-k plots) for both the original and *P1* symmetry settings for every generation in the NSGA-II and –III process. The band gap values are presented if available.

**Table S1.** The effect of the molecular orientation on the DFT-calculated total energy, band gap, and the effective mass for 27 random initial ‘A’-site molecular orientations for  $(\text{NH}_3\text{OH})\text{PbCl}_3$  and  $(\text{CH}_3\text{NH}_3)\text{Cl}$ . Two different symmetry settings were adopted for band structure calculations, Bravais lattice setting in the left side and primitive  $P1$  setting in the right side. The molecules are numbered identically to that shown in Figure S1.

**Table S2.** The DFT-calculated total energy for all the hypothetical MX compounds used for the reaction (formation) energy calculation.

**Table S3.** The DFT-calculated total energy for all the real and hypothetical  $\text{BX}_2$  compounds used for the reaction (formation) energy calculation. Real and hypothetical  $\text{BX}_2$  structures are discerned using colors (blue font for hypothetical).

**Table S4.** The decision variable and objective function values for all the entries belonging to the 1<sup>st</sup> ~ 5<sup>th</sup> generations for NSGA-II.

**Table S5.** The deserted entries (marked in red font) from all ‘A’-site molecule and ‘B’-site atom candidates, which were used for NSGA-II but not for the ensuing NSGA-III.

**Table S6.** The decision variable and objective function values for all the entries belonging to the 1<sup>st</sup> ~ 5<sup>th</sup> generations for NSGA-III.

The data contents in higher resolution will be provided for those who email the corresponding author with reasonable request.

## Supporting Discussion 1

Evidence supporting the apparent-structure-type concept

We introduced 10 different structures belonging to a single apparent-structure-type (#1 in Fig. 2) for a single hypothetical composition of  $\text{CsSnI}_3$  and calculated the total energy and band gap. The following table lists the 10 structures and their total energy and band gap obtained from DFT calculations.

ICSD Coll. Code	Space group	Total energy / f.u. (eV)	$E_g$ (eV)
56472	$Pm\text{-}3m$	-14.0330	0.47
417373	$P4/\text{mmm}$	-14.0330	0.48
109294	$P4mm$	-14.0330	0.48
24515	$Fm\text{-}3m$	-14.0422	0.46
39736	$P2_1/n$	-14.0028	0.48
6061	$I4/\text{mmm}$	-14.0430	0.46
300285	$P4/\text{mbm}$	-14.0366	0.48
69995	$P4/\text{mbm}$	-14.0133	0.48
243734	$Pnma$	-13.9569	0.48
410977	$P3_2$	-14.0026	0.49

We set up input model structures based on the Bravais lattice except for the structures 39736 ( $P2_1/n$ ), 69995 ( $P4/\text{mbm}$ ), and 410977 ( $P3_2$ ), for which the primitive cells were used. The structure relaxation was implemented under the same convergence conditions that we used for the NSGA-II and –III processes. When  $\text{CsSnI}_3$  stoichiometry was applied, these ten hypothetical structures gave almost identical total energy and band gap values irrespective of the choice of symmetry in the initial input model structure. This implies that an orthodox symmetry classification would by no means be suitable when the structure relaxation was implemented with no constraints. This indirectly reflects that the newly suggested ‘apparent-structure-type’ concept is plausible as far as the structure relaxation with no constraints is of concern.

On these grounds, if some potential candidates belonging to this apparent-structure-type were predicted by the NSGA-II and –III process, they would crystallize either into one of these 10 structures or into none of them, but the overall appearance of the predicted structure might be similar to this apparent-structure-type.

## Supporting Discussion 2

### Symmetry setting for band structure

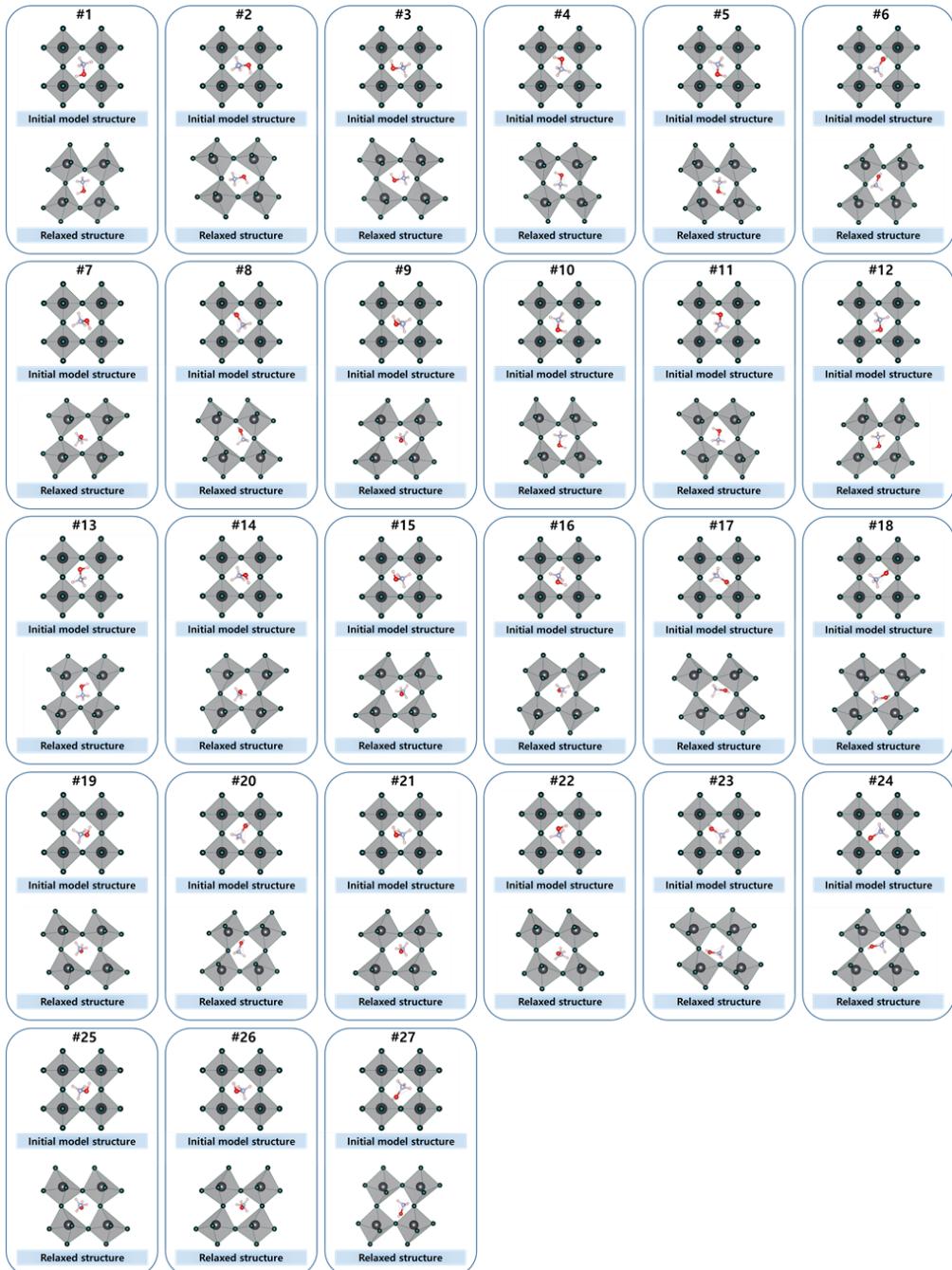
$\text{Cs}_4\text{PbCl}_6$  (*R*-3c) was nominated as a model system that could be used to examine the effect that symmetry setting could exert on the band structure (and DOS) calculation. We prepared three different CHGCAR files originating from three different symmetry settings for the initial input model structures used for structure relaxation. The first input model structure was constructed using the original Bravais lattice (*R*-3c), which was then structure-relaxed with a strict symmetry restriction adhering to the original symmetry. The second model was the same as the first with the exception of being structure-relaxed with no symmetry restriction, which means that all atomic positions, volume and shape, were free to be adjusted with no constraints. The third input model structure was constructed using a primitive cell of the original Bravais lattice, which was then structure-relaxed with no constraints. Thereafter, we secured three different CHGCAR files originating from the above-described three models. Also, the total energy values for the relaxed structures from these three input model structures were almost identical, as shown below.

Input model Space group	VASP E. / f.u	$E_g$ _Bravais (eV)	$E_g$ _P1 (eV)	$E_g$ _PP1 (eV)
<i>R</i> -3c (Bravais)	-75.333	4.29	4.28	4.28
<i>P</i> 1	-75.333	4.27	4.27	4.27
Primitive <i>P</i> 1 (PP1)	-75.334	4.28	4.28	4.28

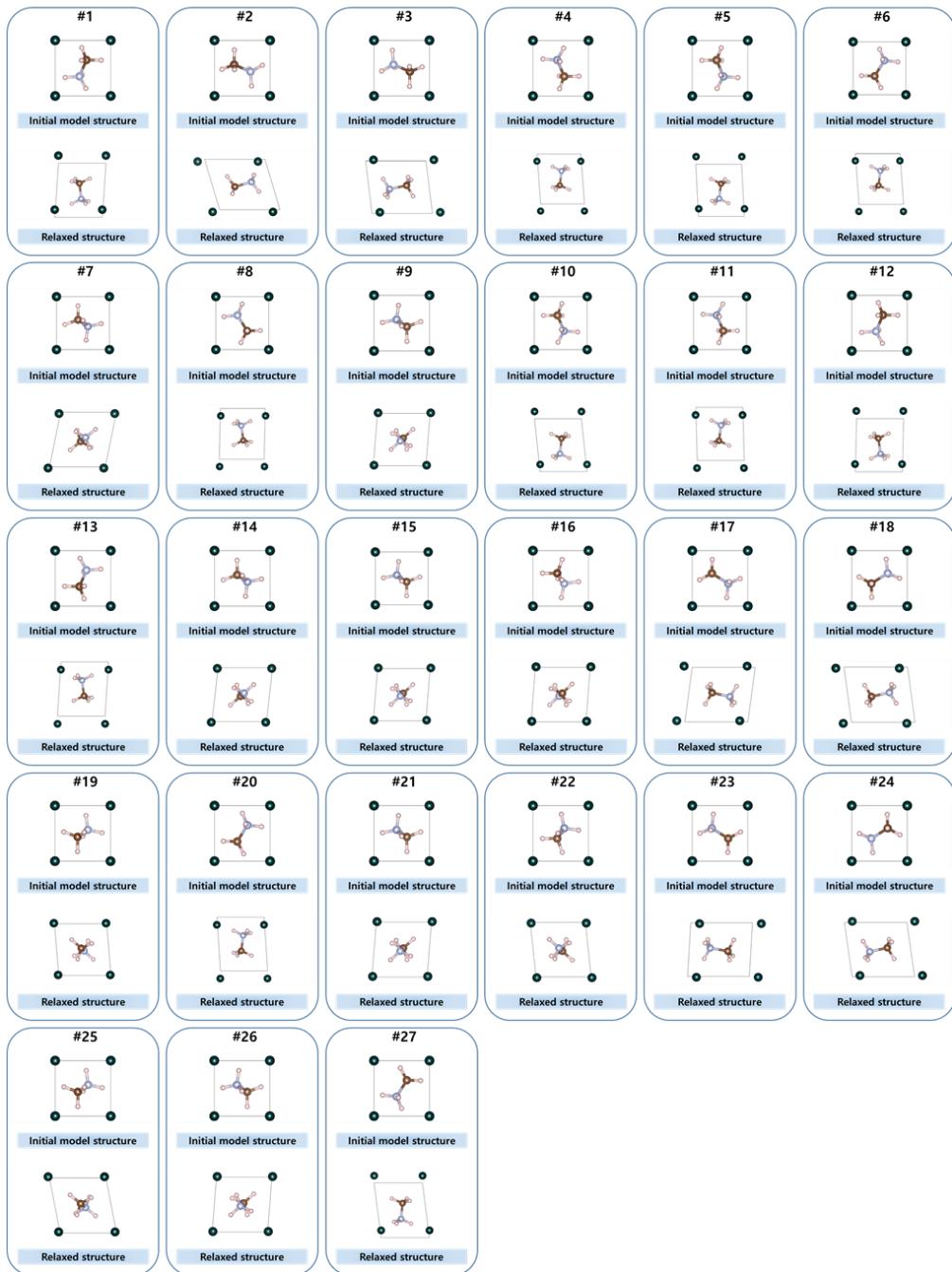
Nine band structures were prepared from the above-described three CHGCAR files by incorporating three symmetry settings per each CHGCAR file. The above table lists the nine band gap values. All the band gaps presented in the above table are similar, which indicates that the symmetry setting would never have great influence on either the self-consistent run for CHGCAR or the ensuing non-self-consistent run for band-structure calculation.

**Fig. S1**

**27 Structures of  $(\text{NH}_3\text{OH})\text{PbCl}_3$**



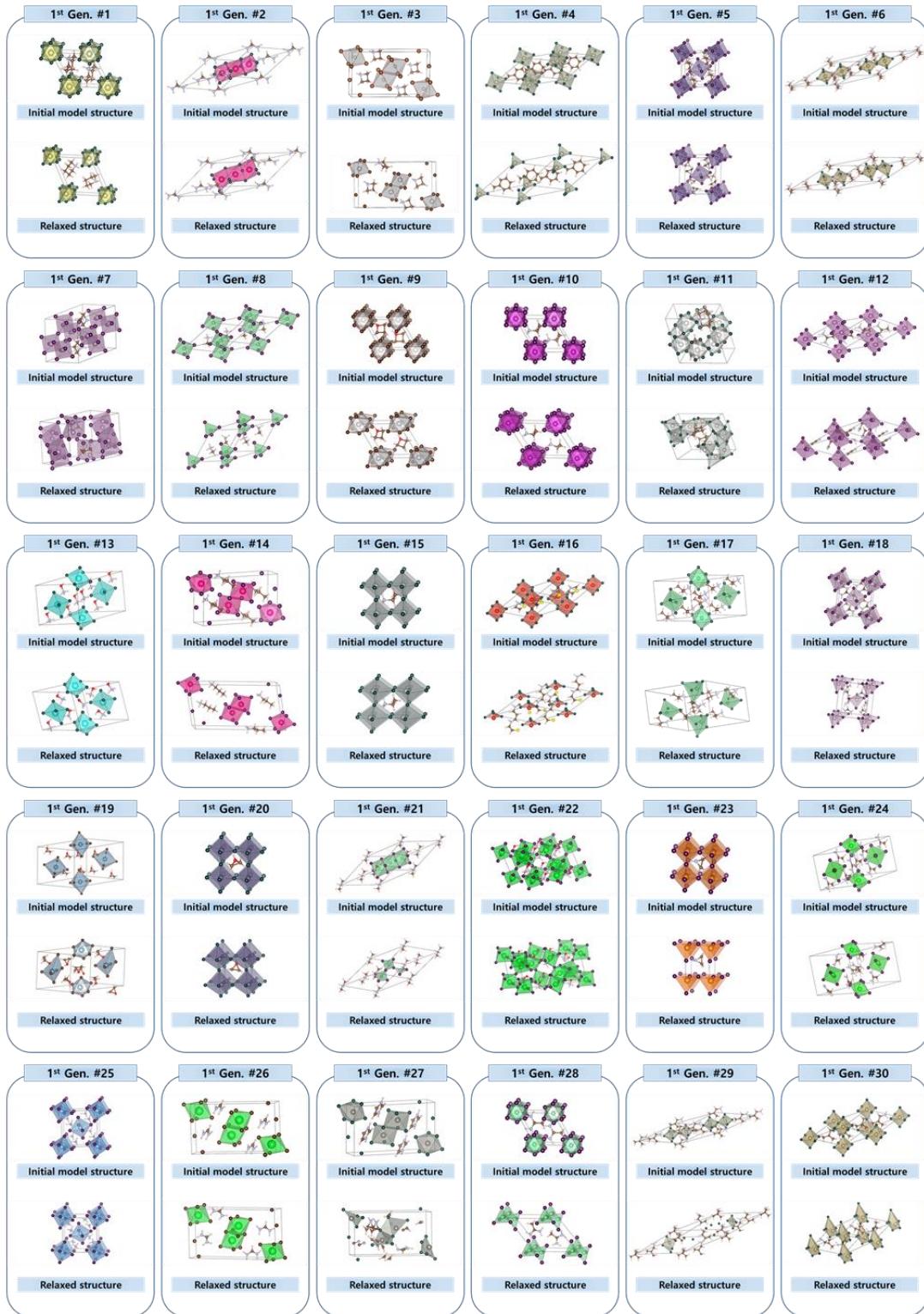
## 27 Structures of $(\text{CH}_3\text{NH}_3)\text{Cl}$



**Figure S1.** The 27 different molecular arrangements for both  $(\text{NH}_3\text{OH})\text{PbCl}_3$  and  $(\text{CH}_3\text{NH}_3)\text{Cl}$  before the DFT-based structure relaxation, and their resultant orientations after the structure relaxation. The randomly located 'A'-site molecule reorients during the DFT-based structure relaxation. The 27 random initial orientations achieved their final relaxed structures for both  $(\text{NH}_3\text{OH})\text{PbCl}_3$  and  $(\text{CH}_3\text{NH}_3)\text{Cl}$ .

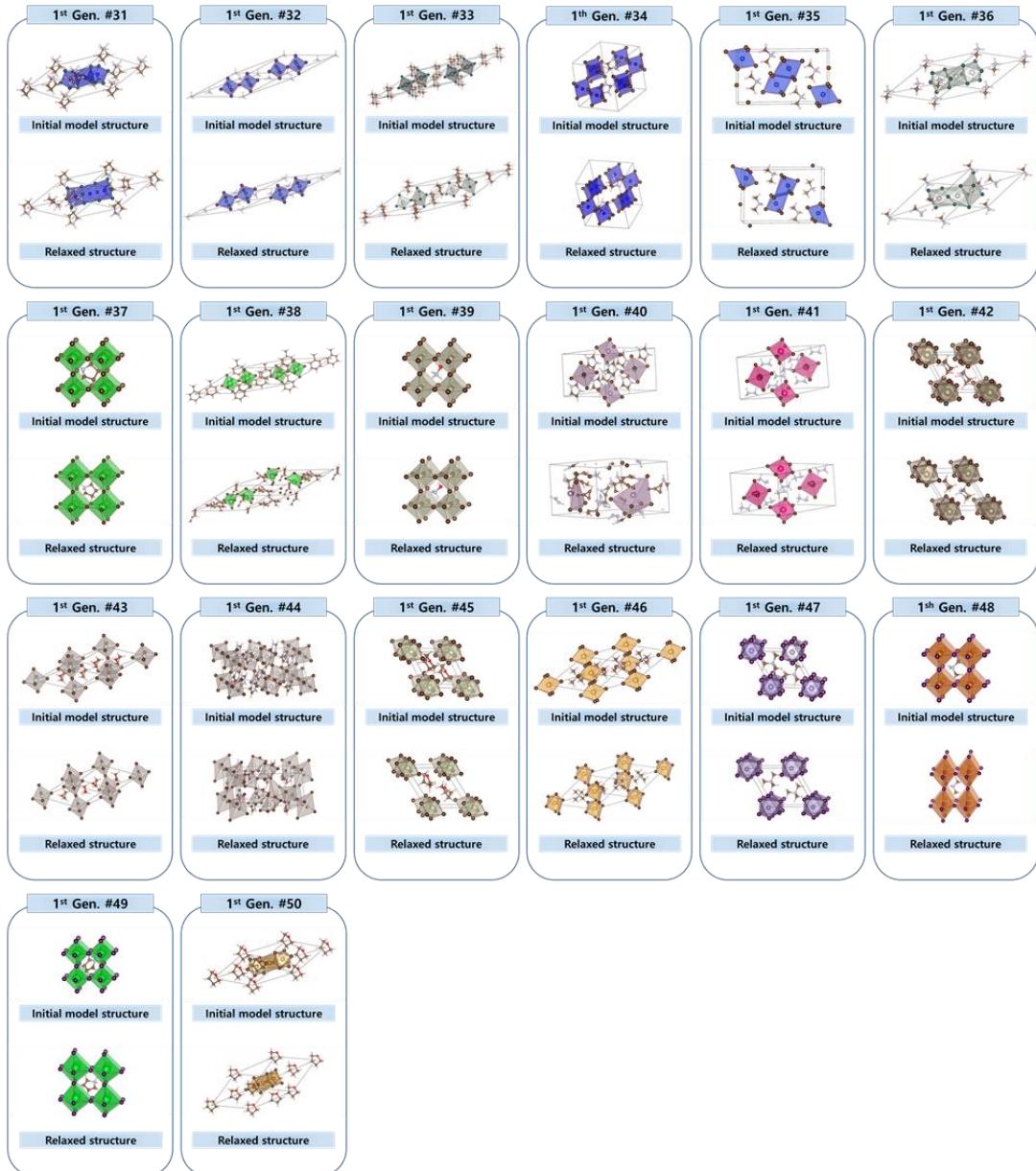
**Fig. S2**

**NSAG-II 1<sup>st</sup> Generation Input model / DFT-relaxed structures**



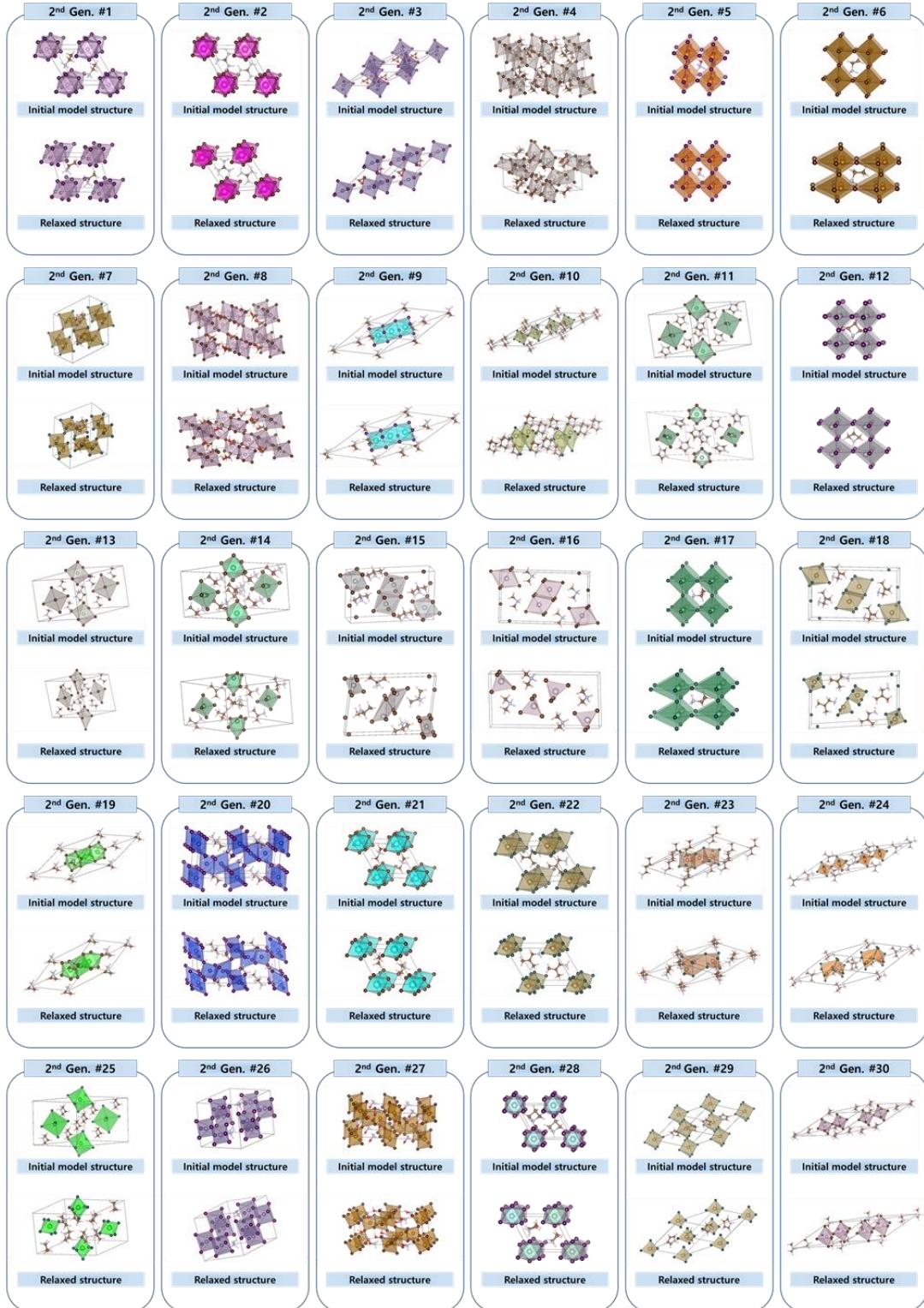
**Fig. S2**

**NSAG-II 1<sup>st</sup> Generation Input model / DFT-relaxed structures**



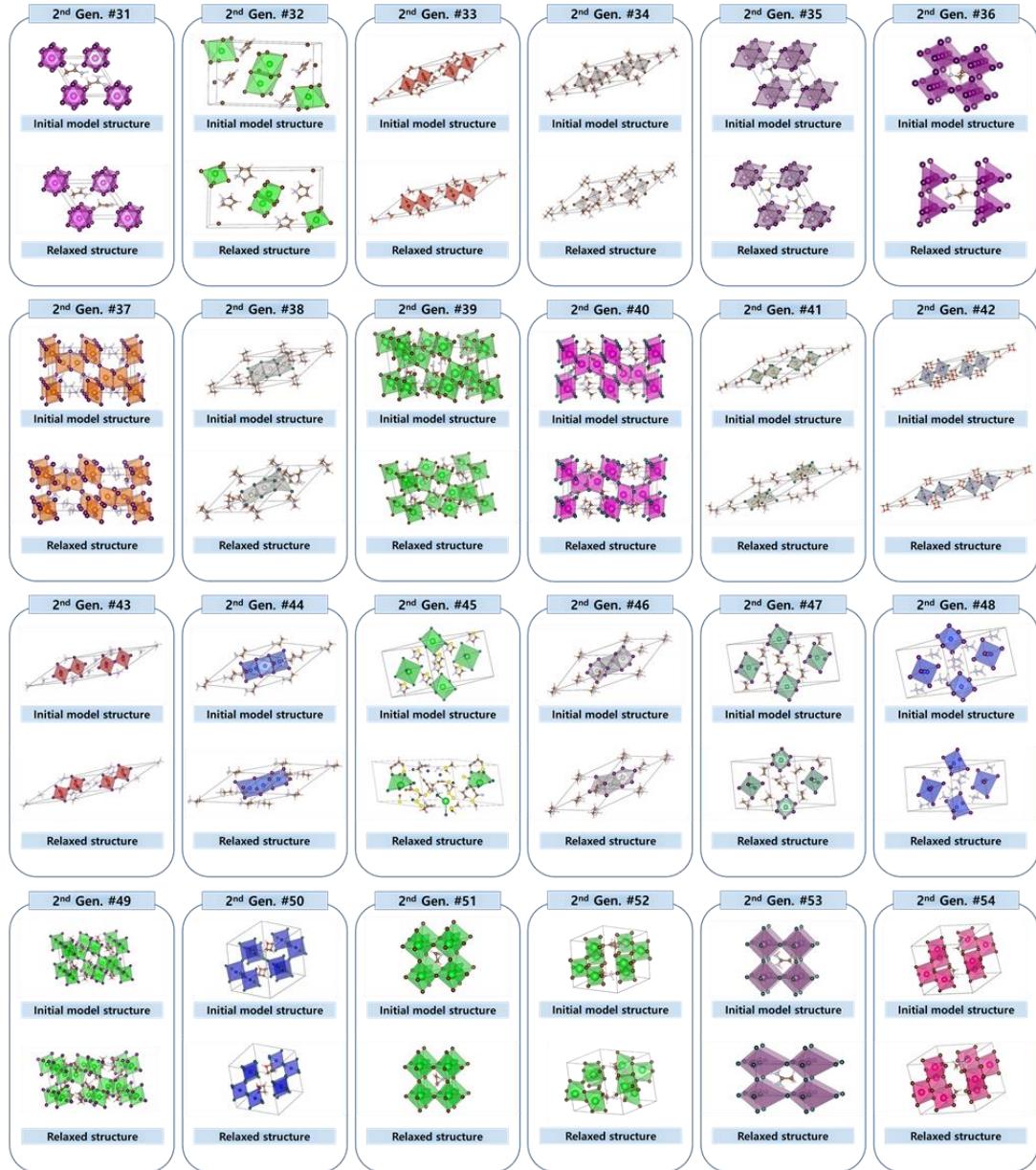
**Fig. S2**

### NSAG-II 2<sup>nd</sup> Generation Input model / DFT-relaxed structures



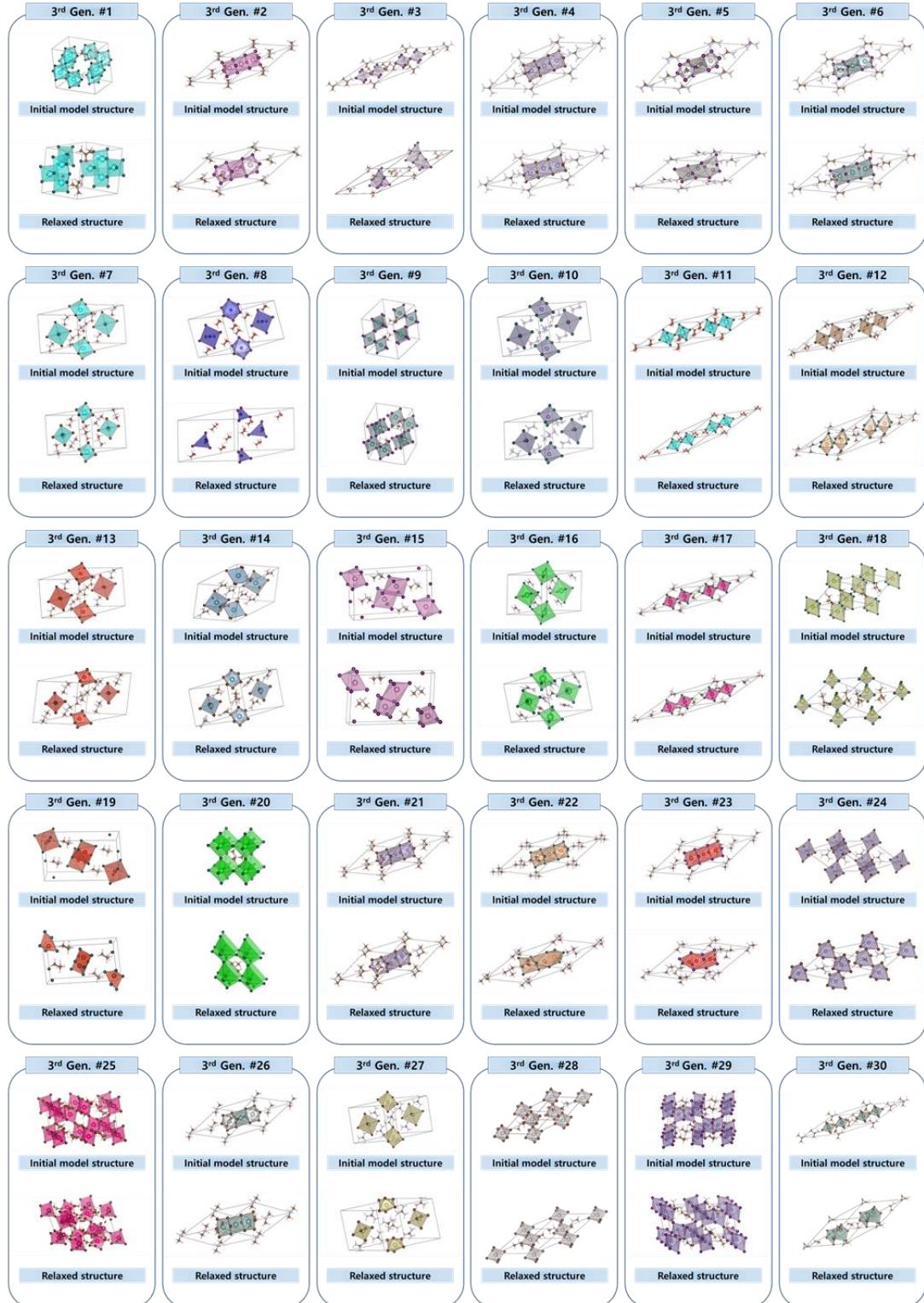
**Fig. S2**

**NSAG-II 2<sup>nd</sup> Generation Input model / DFT-relaxed structures**



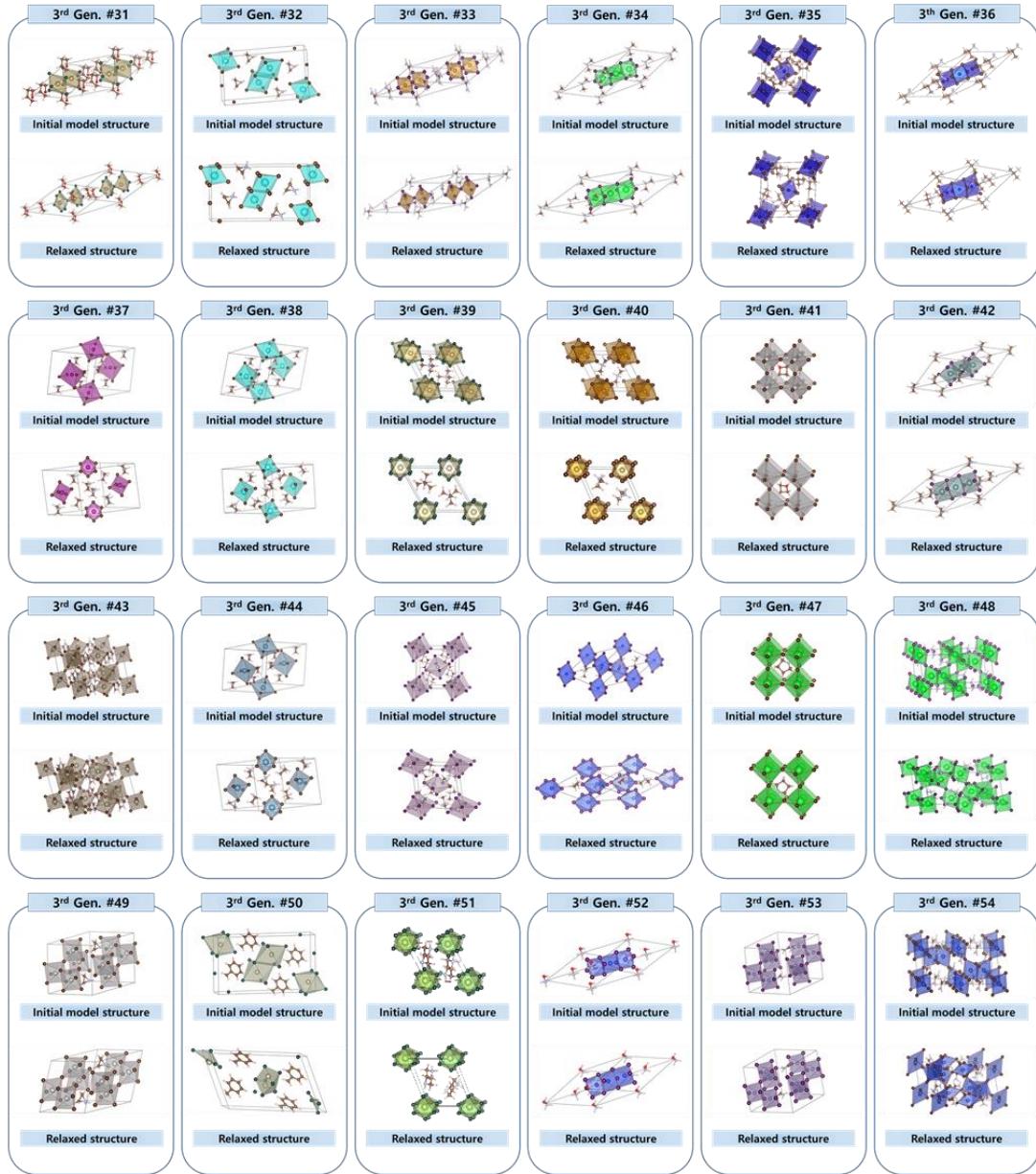
**Fig. S2**

**NSAG-II 3<sup>rd</sup> Generation Input model / DFT-relaxed structures**



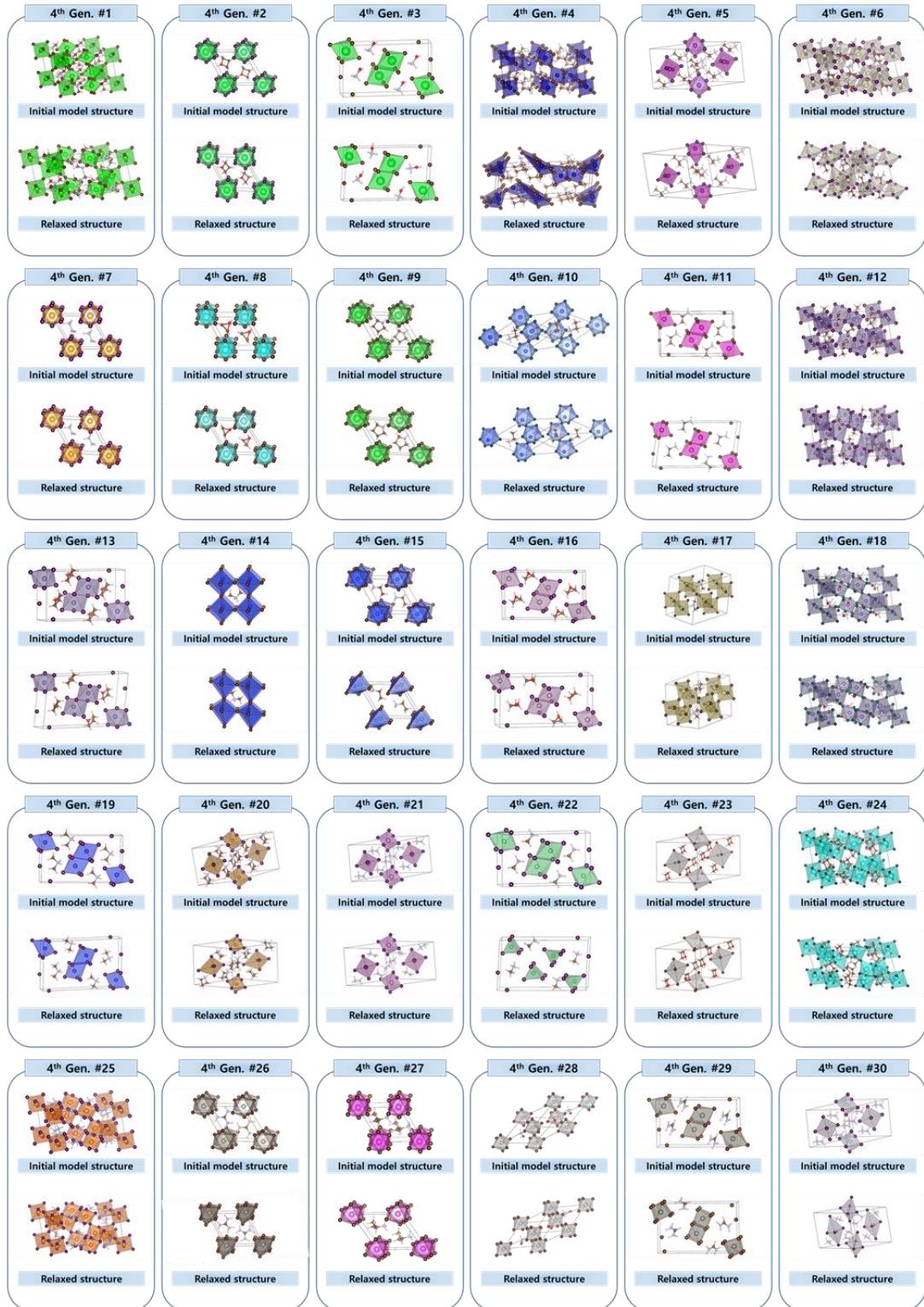
**Fig. S2**

**NSAG-II 3<sup>rd</sup> Generation Input model / DFT-relaxed structures**



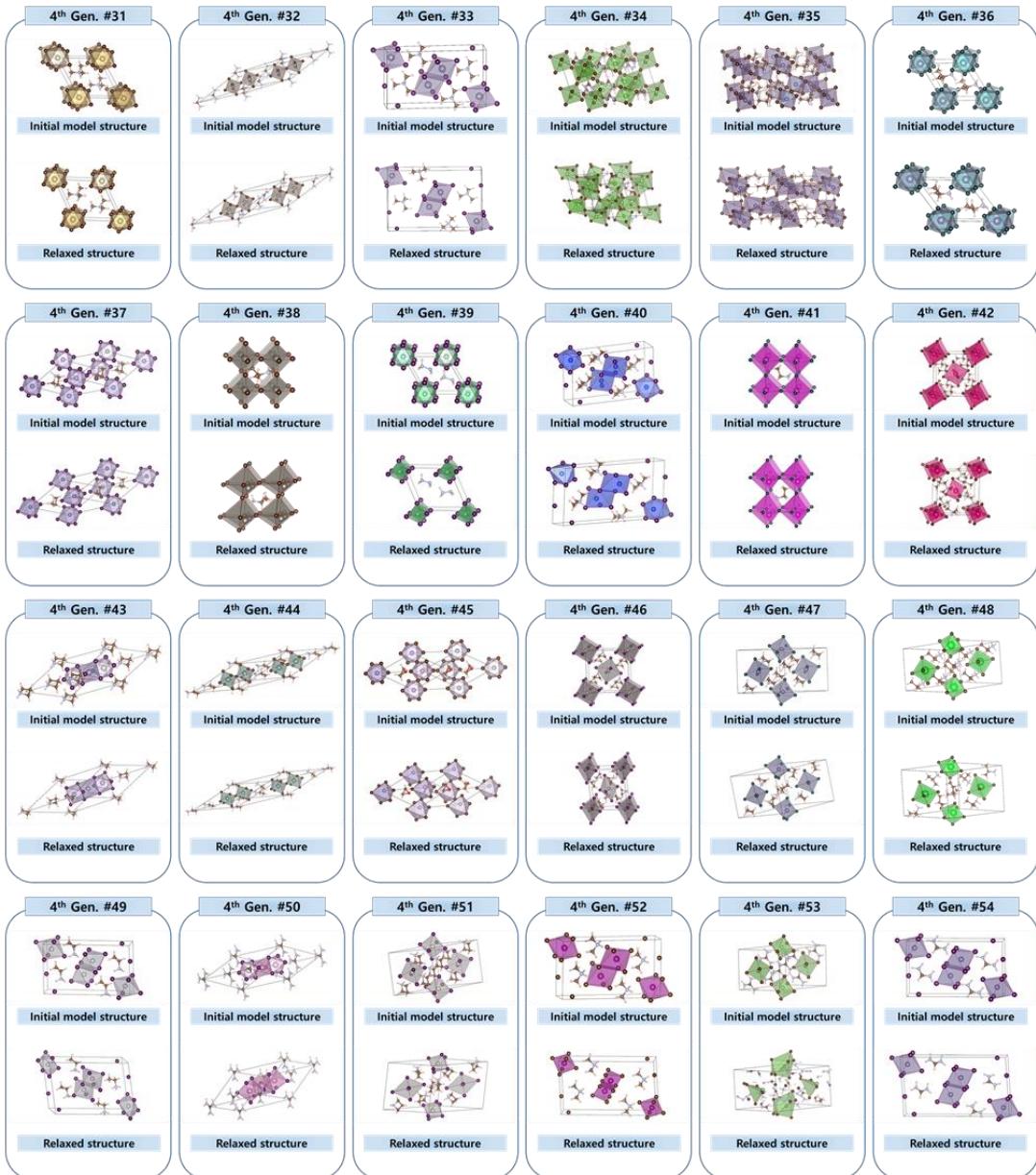
**Fig. S2**

**NSAG-II 4<sup>th</sup> Generation Input model / DFT-relaxed structures**



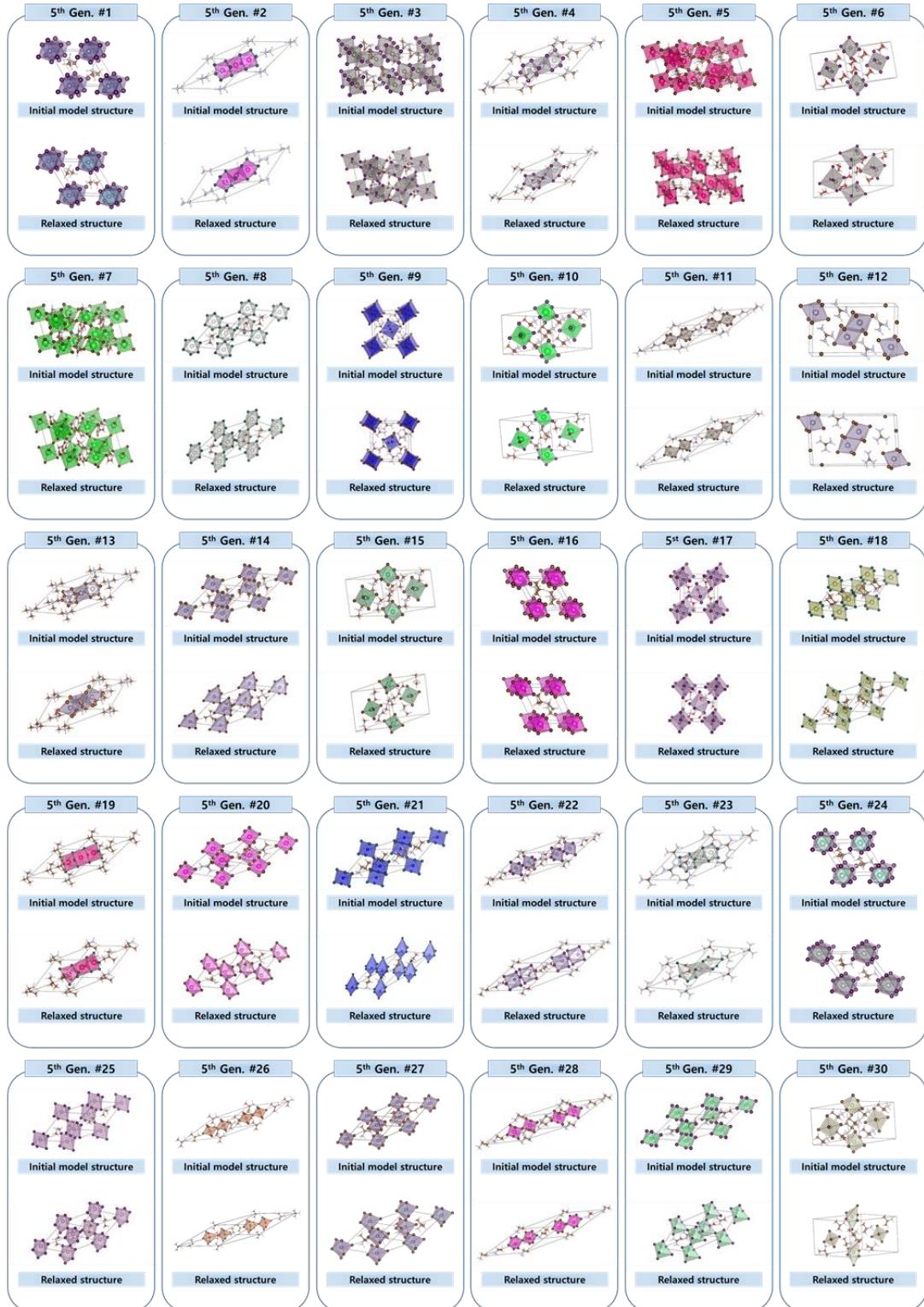
**Fig. S2**

**NSAG-II 4<sup>th</sup> Generation Input model / DFT-relaxed structures**



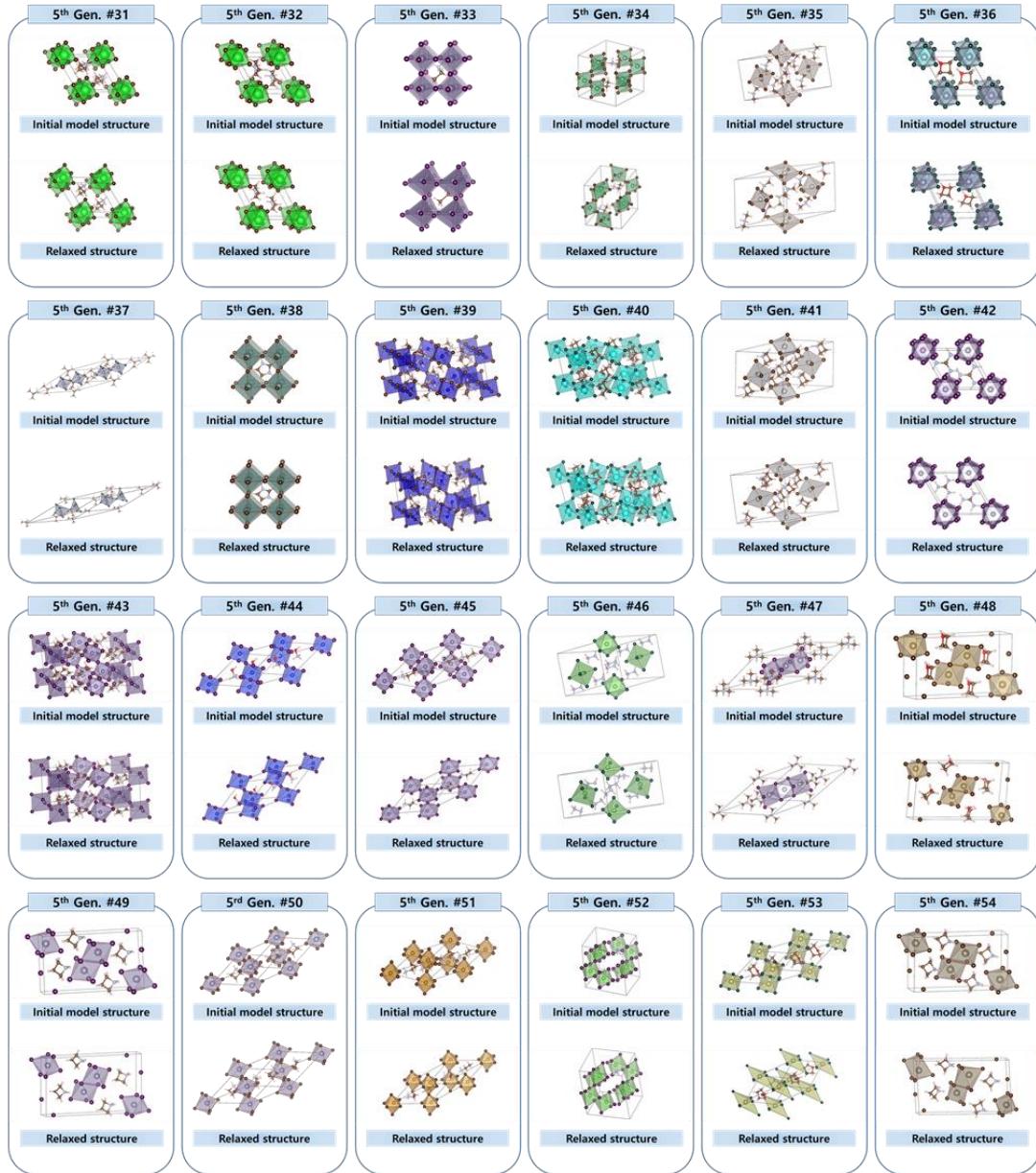
**Fig. S2**

**NSAG-II 5<sup>th</sup> Generation Input model / DFT-relaxed structures**



**Fig. S2**

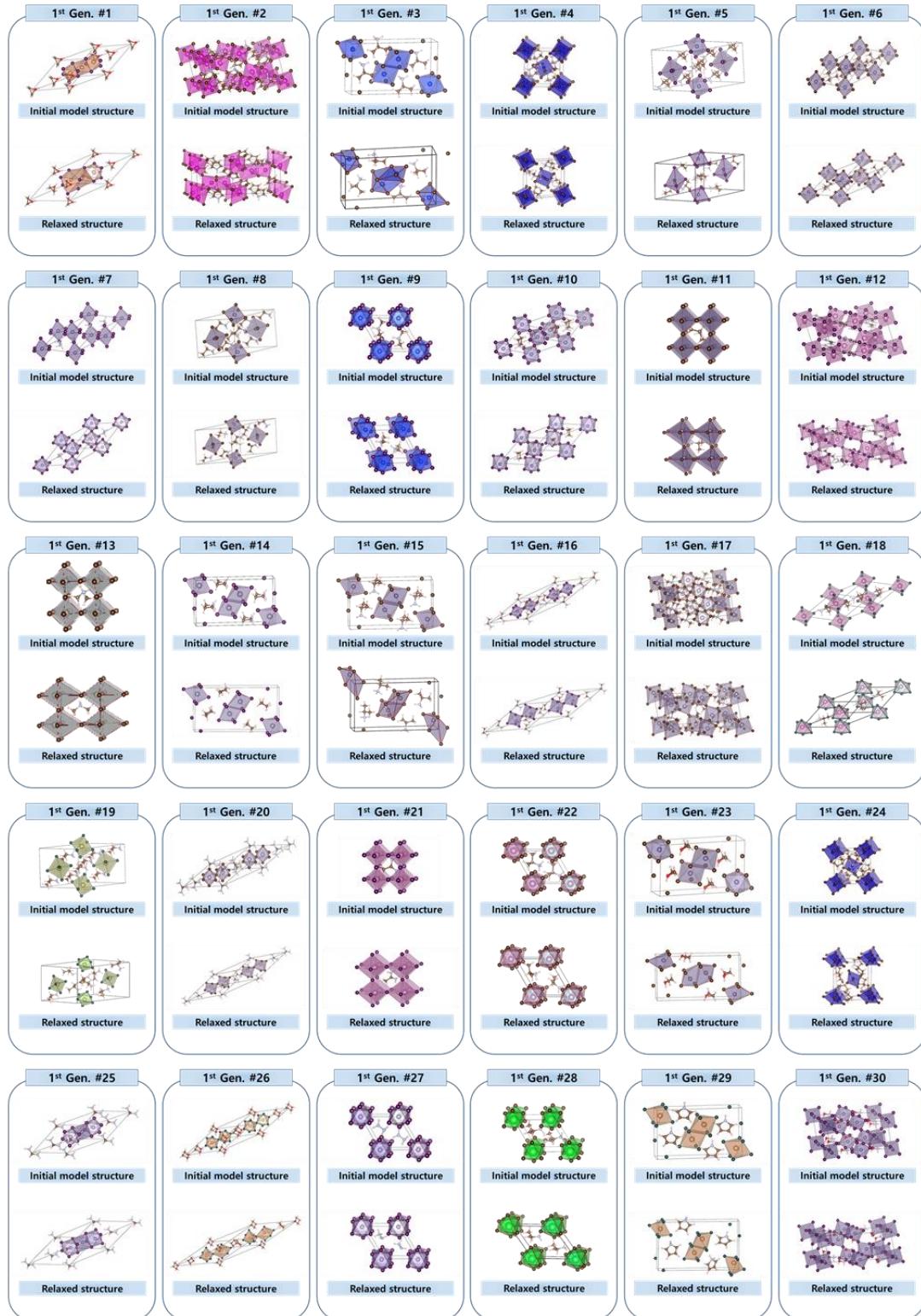
**NSAG-II 5<sup>th</sup> Generation Input model / DFT-relaxed structures**



**Figure S2.** Input model structures and their DFT-relaxed structures (from the 1<sup>st</sup> to 5<sup>th</sup> generations) used for NSGA-II.

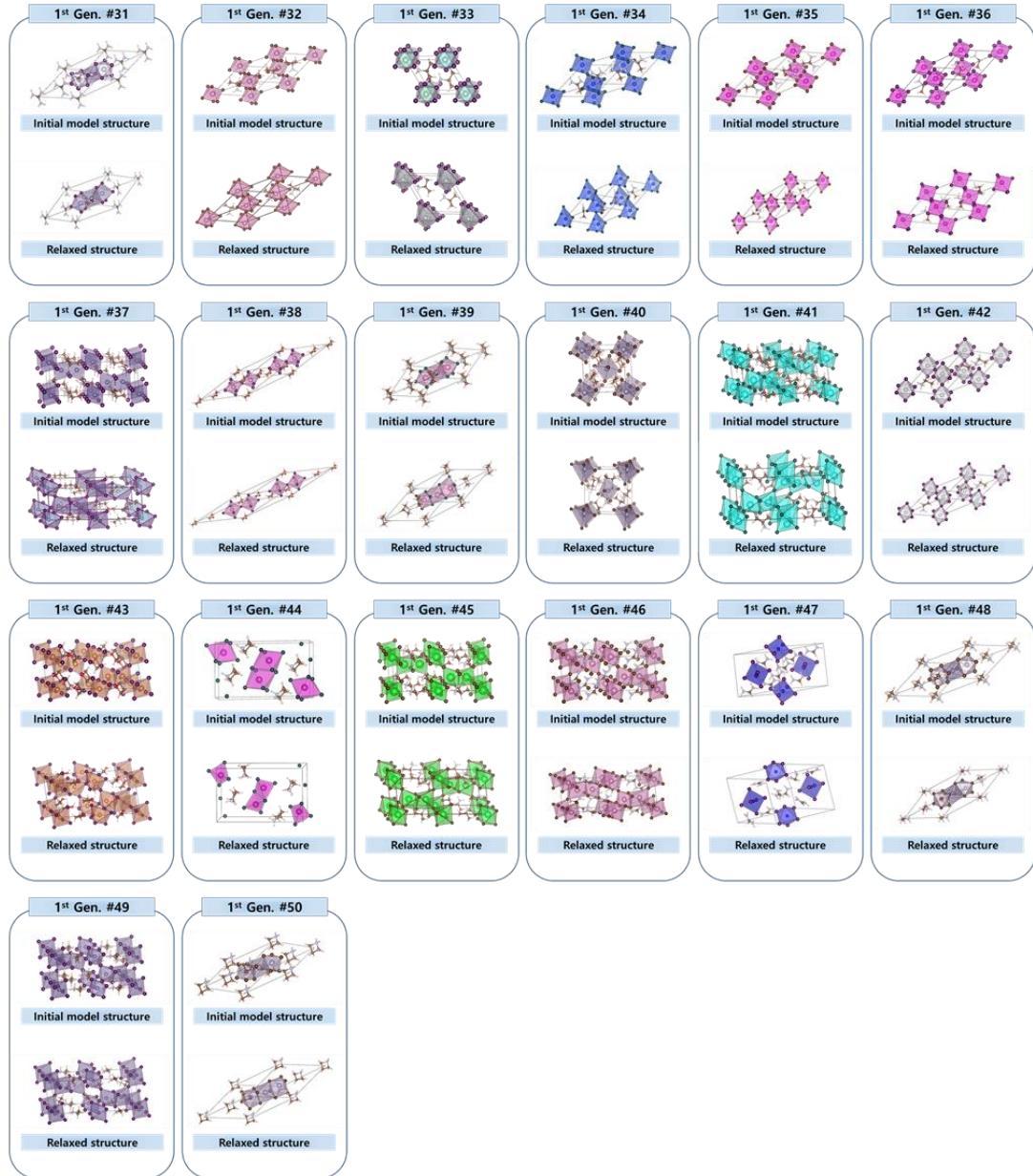
**Fig. S3**

### NSAG-III 1<sup>st</sup> Generation Input model / DFT-relaxed structures



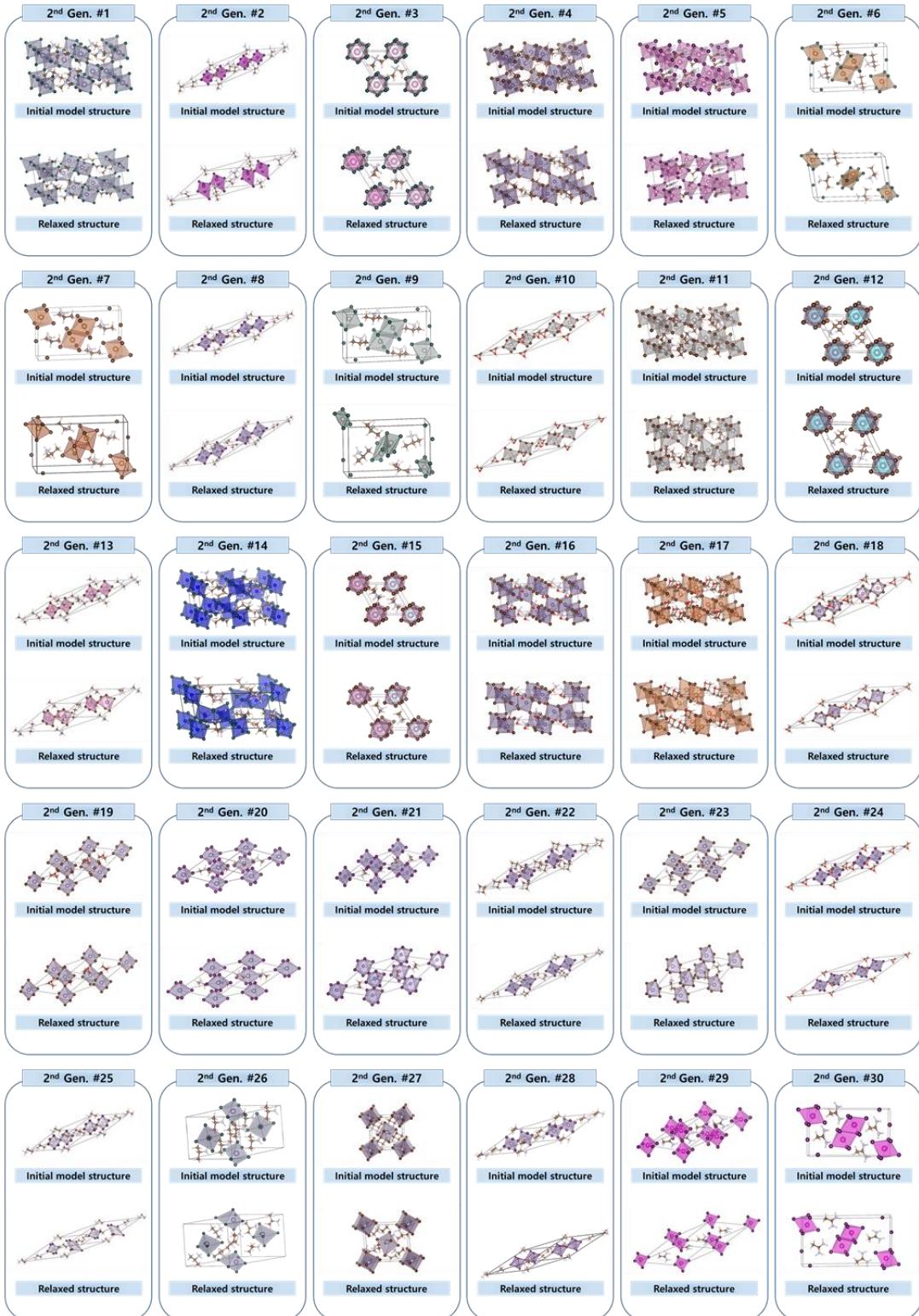
**Fig. S3**

**NSAG-III 1<sup>st</sup> Generation Input model / DFT-relaxed structures**



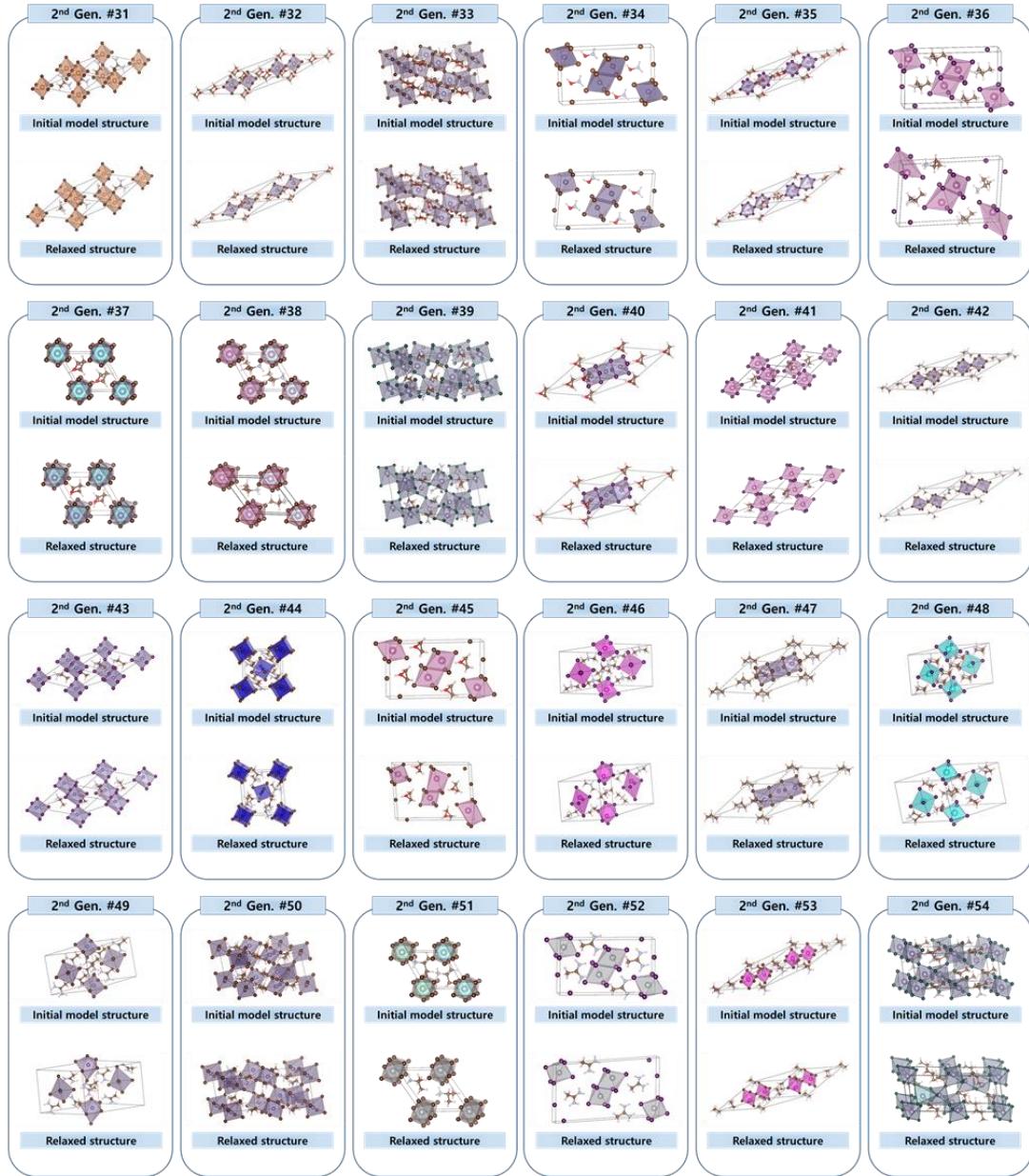
**Fig. S3**

**NSAG-III 2<sup>nd</sup> Generation Input model / DFT-relaxed structures**



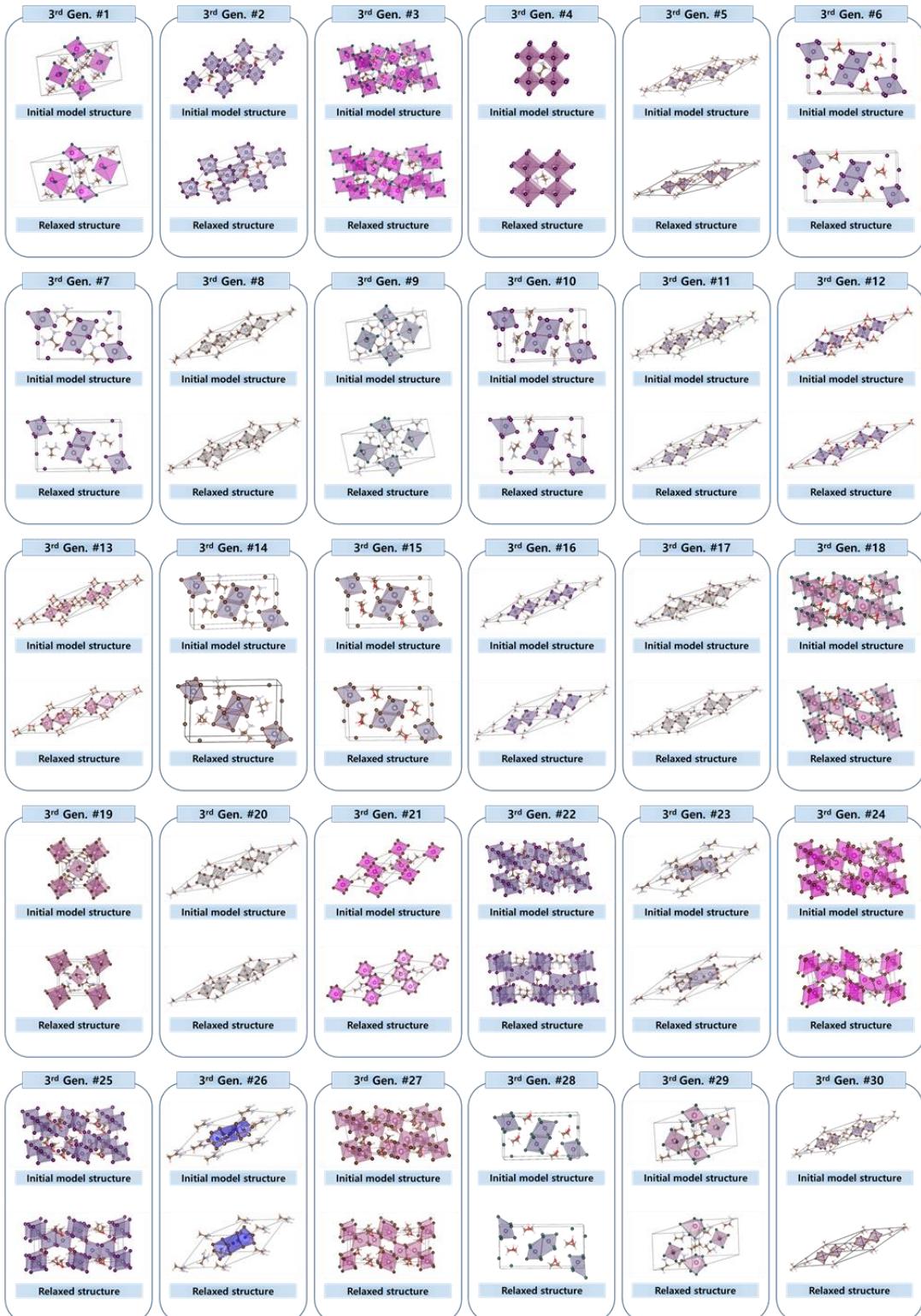
**Fig. S3**

**NSAG-III 2<sup>nd</sup> Generation Input model / DFT-relaxed structures**



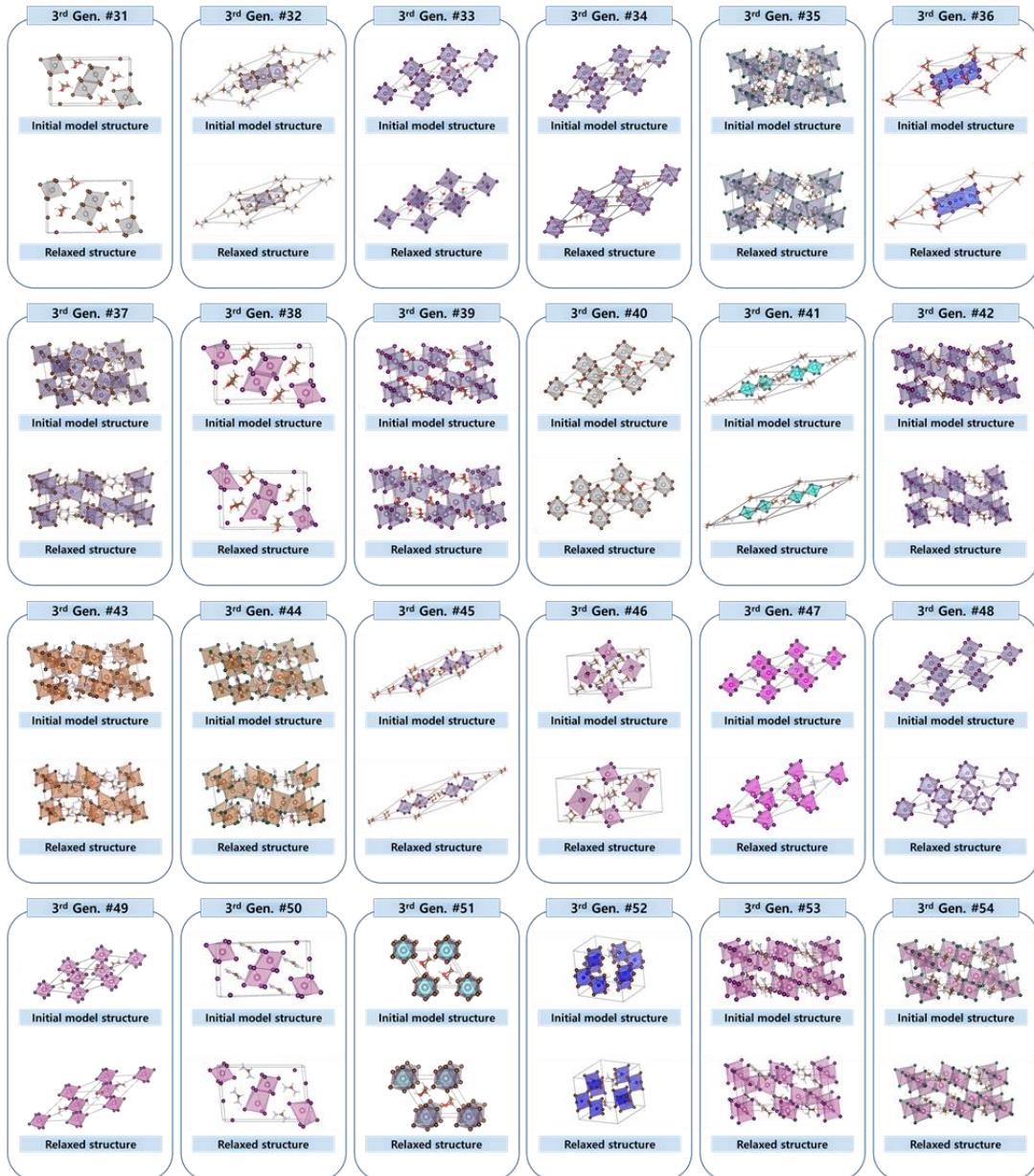
**Fig. S3**

**NSAG-III 3<sup>rd</sup> Generation Input model / DFT-relaxed structures**



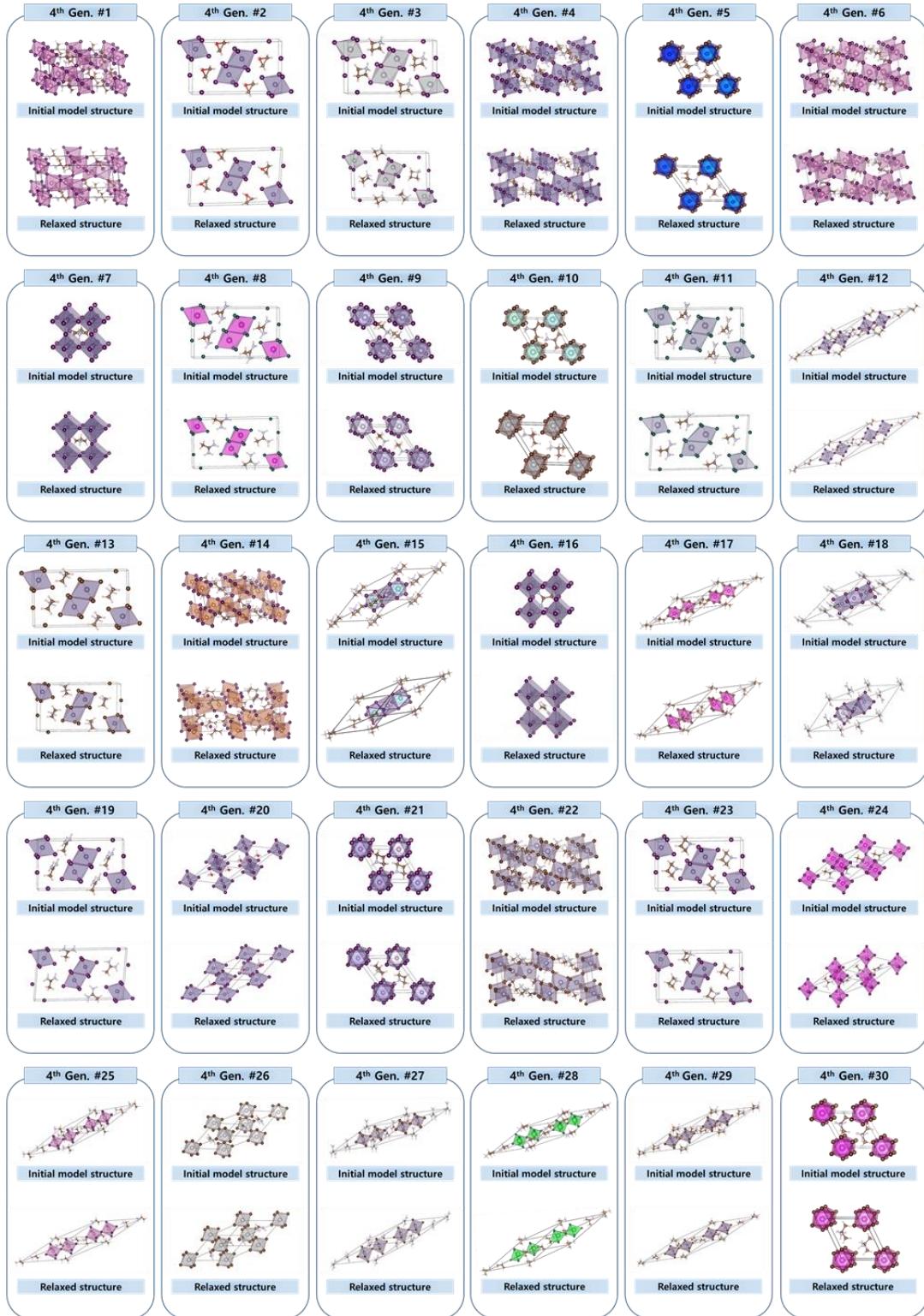
**Fig. S3**

**NSAG-III 3<sup>rd</sup> Generation Input model / DFT-relaxed structures**



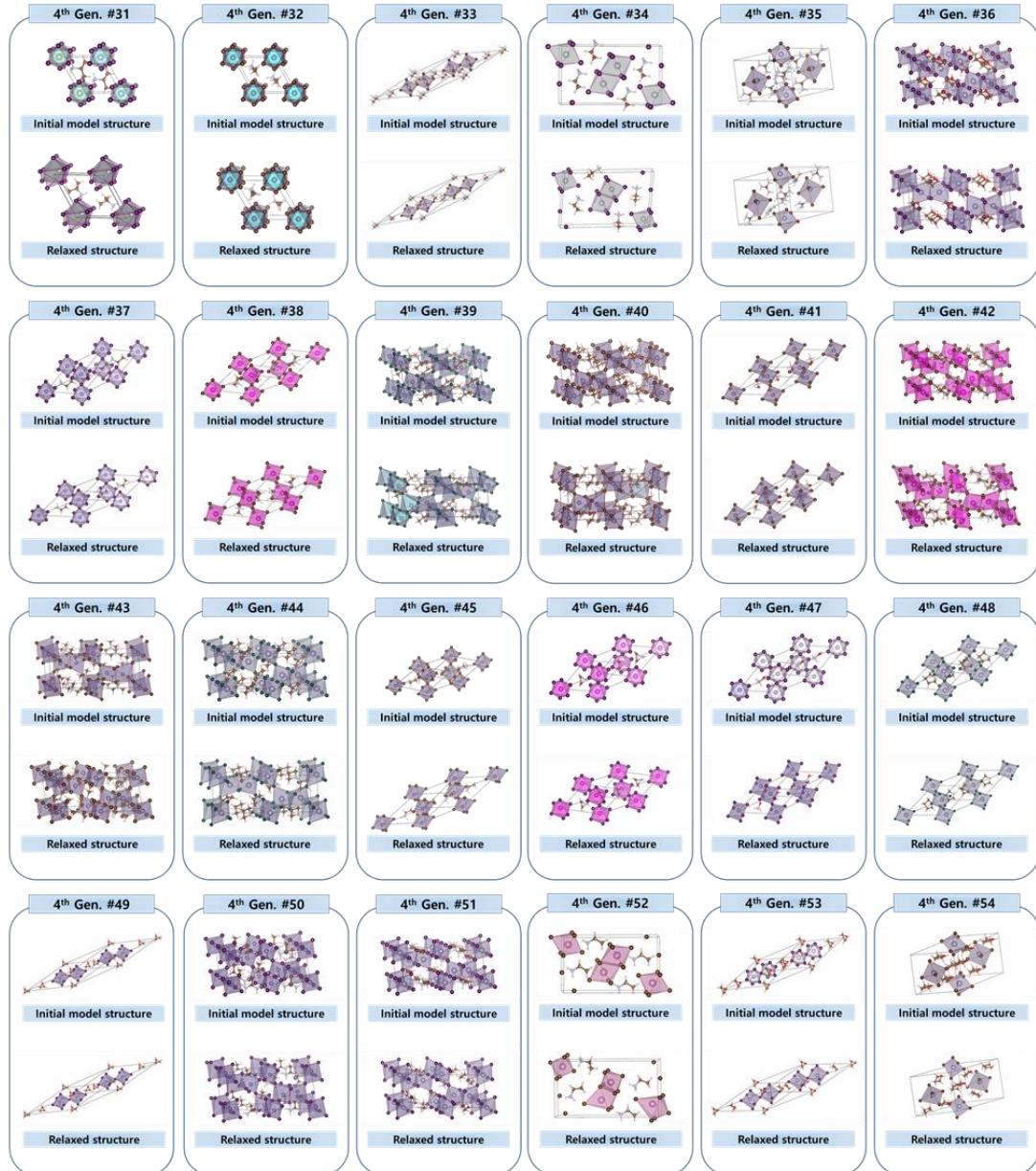
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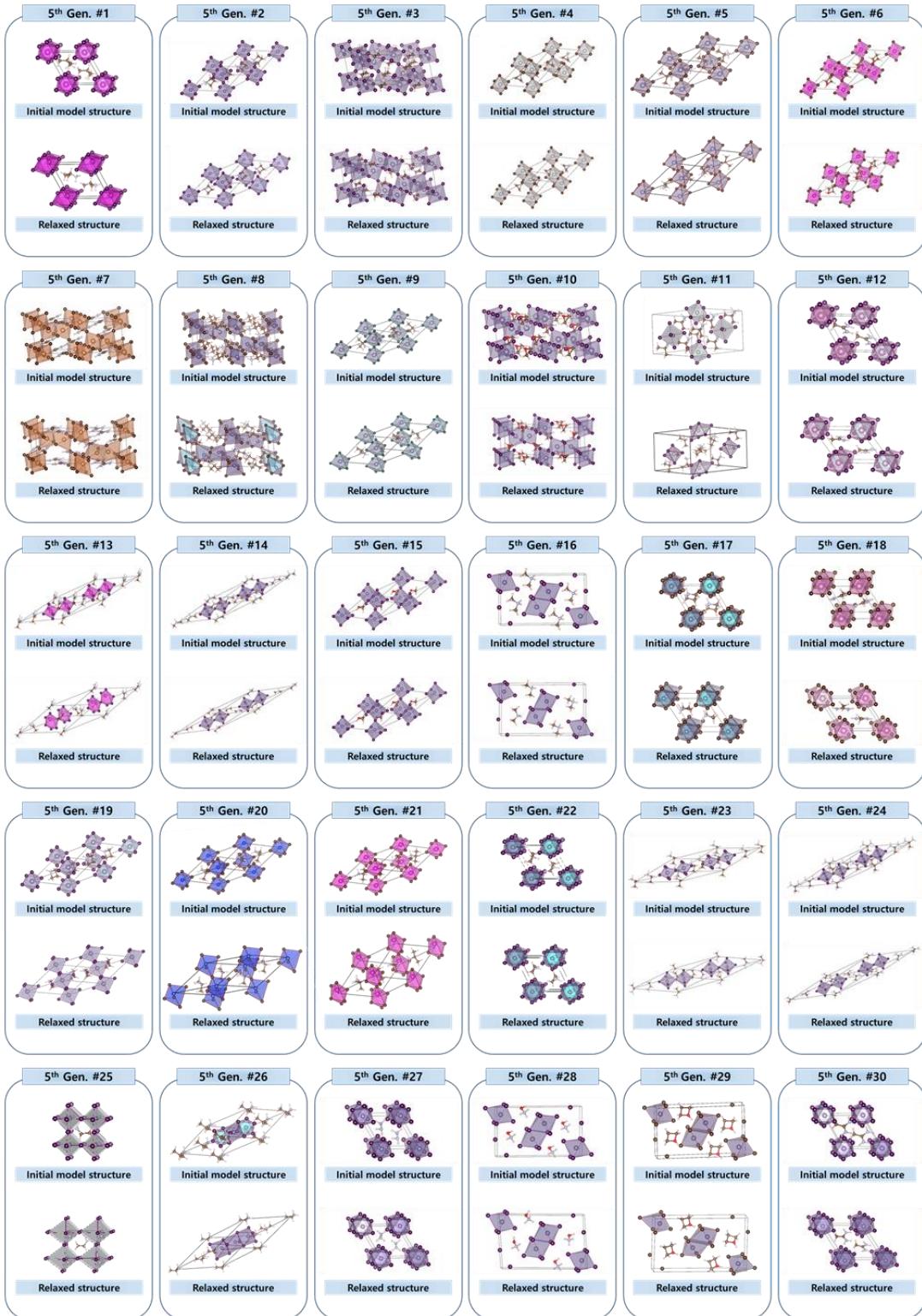
**Fig. S3**

**NSAG-III 4<sup>th</sup> Generation Input model / DFT-relaxed structures**



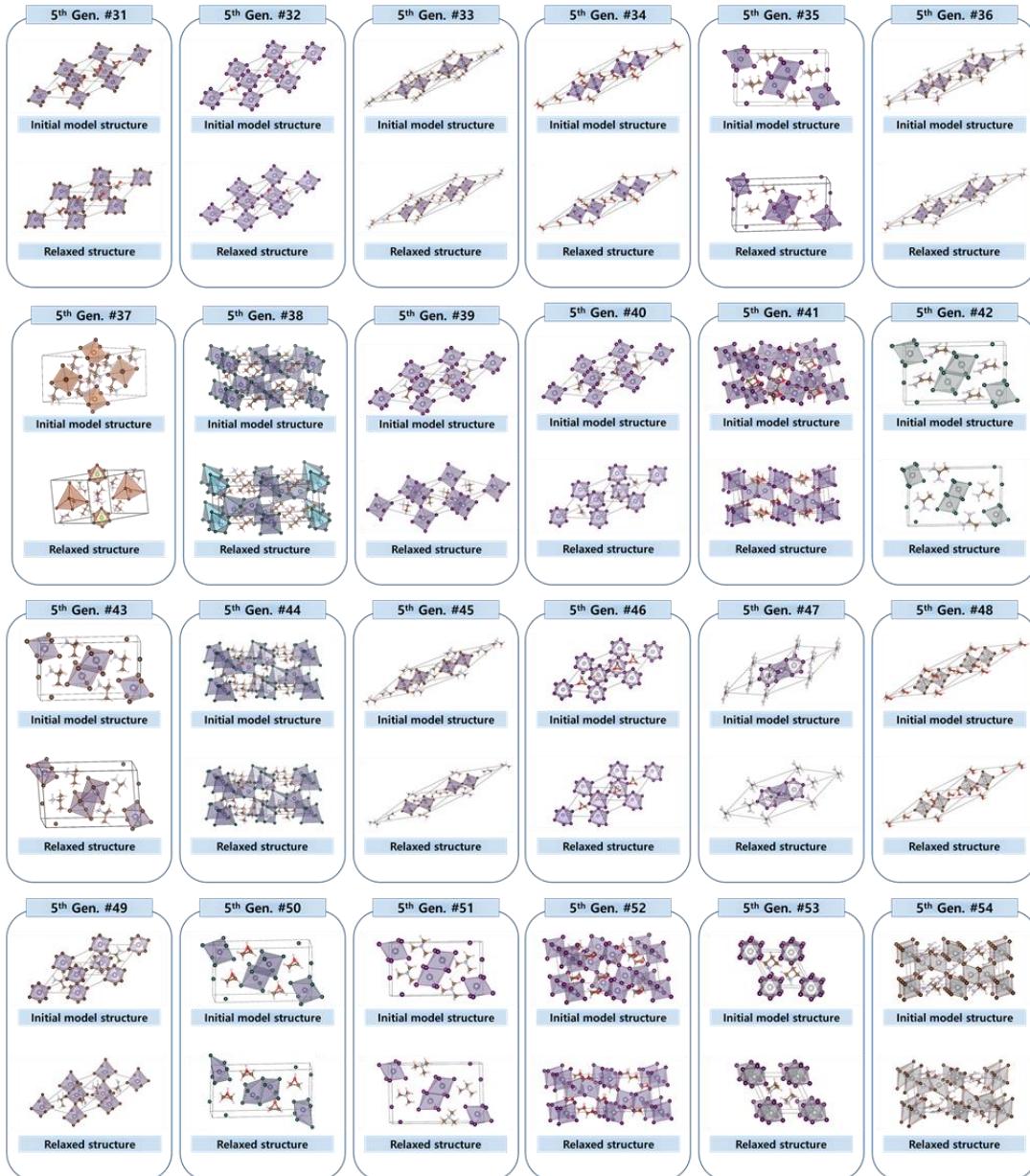
**Fig. S3**

**NSAG-III 5<sup>th</sup> Generation Input model / DFT-relaxed structures**



**Fig. S3**

**NSAG-III 5<sup>th</sup> Generation Input model / DFT-relaxed structures**



**Figure S3.** Input model structures and the DFT-relaxed structures (from the 1<sup>st</sup> to 5<sup>th</sup> generations) used for NSGA-III.

**Fig.4 (page 27 – 66)**



## NSAG-II 1<sup>st</sup> Generation

Original symmetry setting

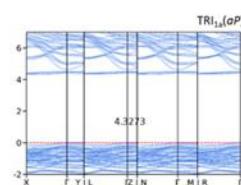
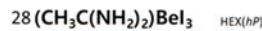
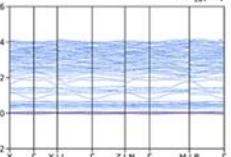
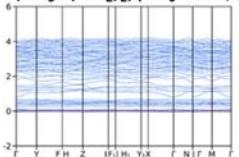
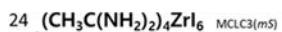
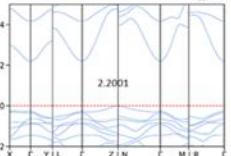
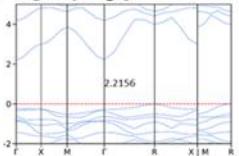
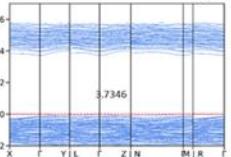
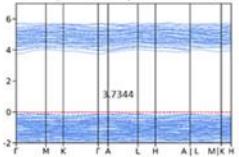
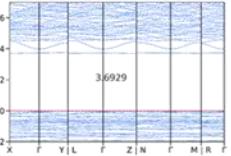
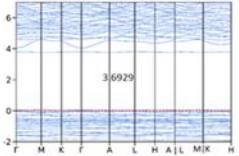
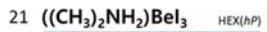
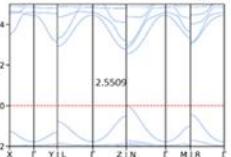
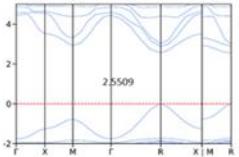
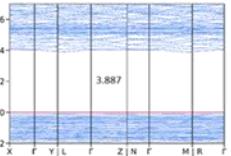
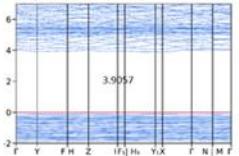
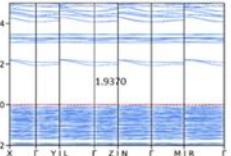
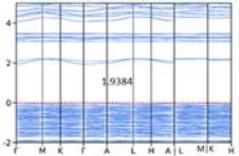
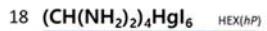
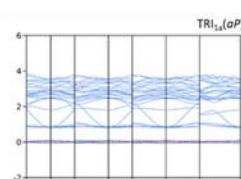
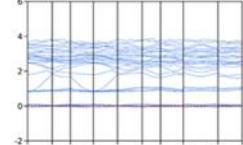


*P1* setting

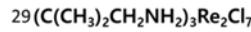
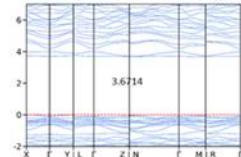
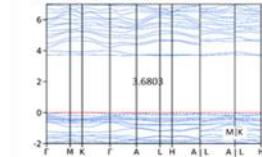
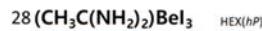
Failure

Original symmetry setting

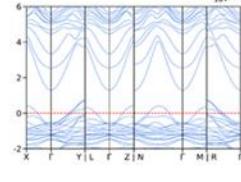
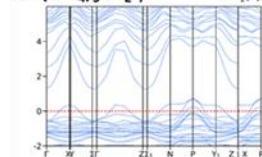
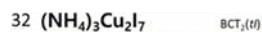
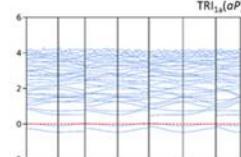
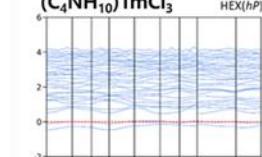
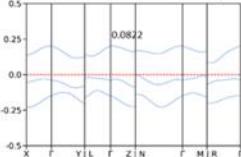
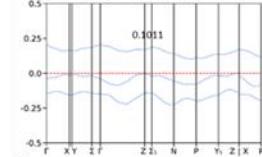
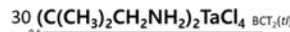
*P1* setting



Failure



Failure



## NSAG-II 1<sup>st</sup> Generation

Original symmetry setting

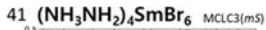


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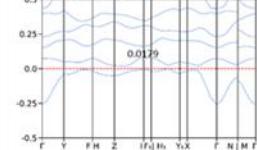
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Original symmetry setting

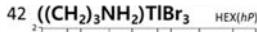
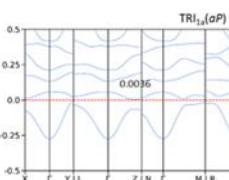
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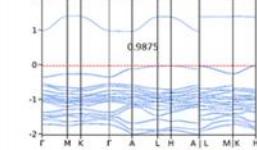
$TRI_{13}(oP)$



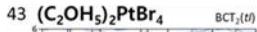
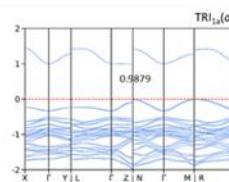
$TRI_{13}(oP)$



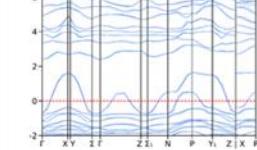
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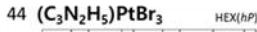
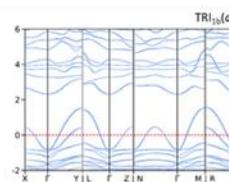
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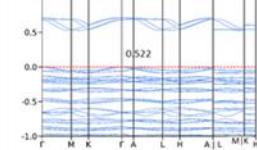
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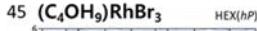
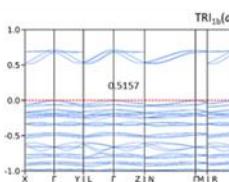
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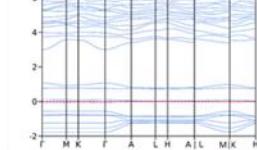
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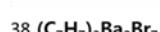
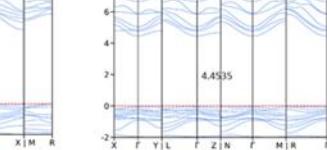
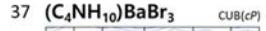
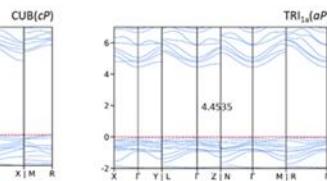
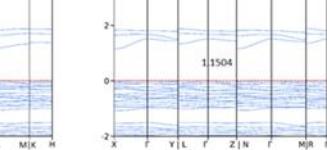
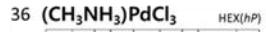
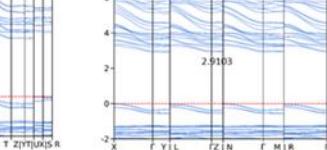
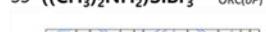
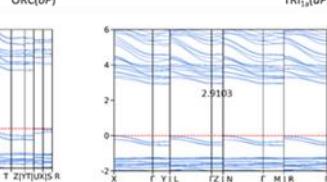
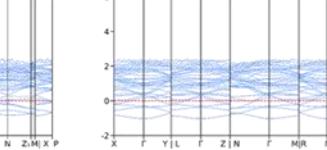
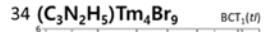
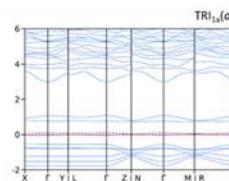
$TRI_{13}(oP)$



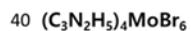
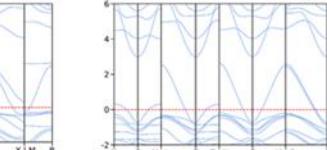
$TRI_{13}(oP)$



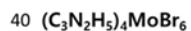
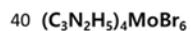
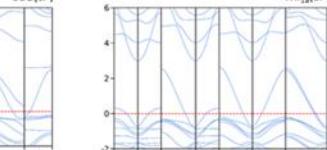
$TRI_{13}(oP)$



Failure

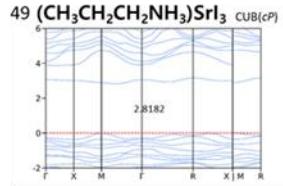


Failure

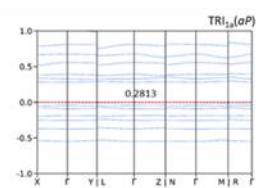
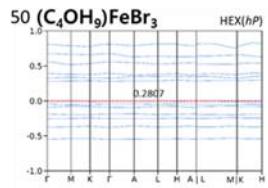
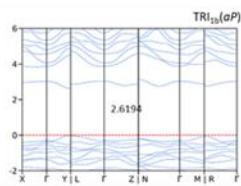


## NSAG-II 1<sup>st</sup> Generation

Original symmetry setting



$P1$  setting



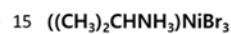
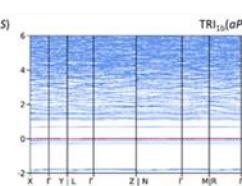
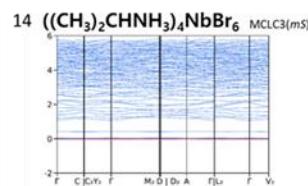
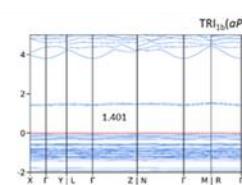
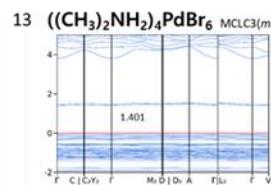
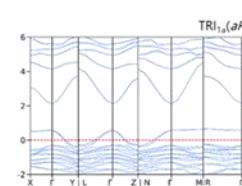
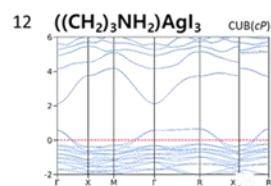
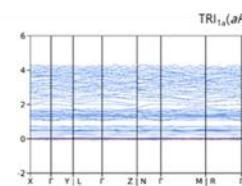
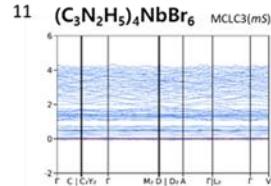
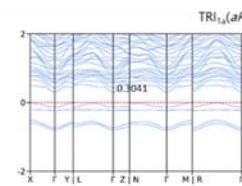
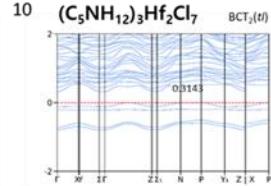
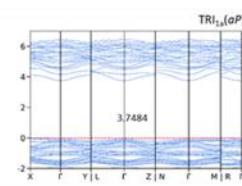
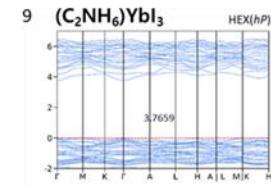
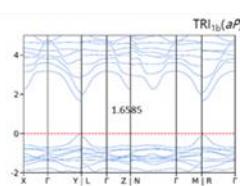
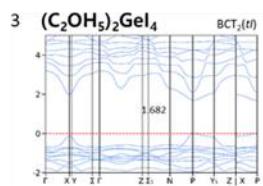
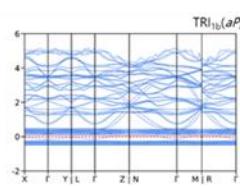
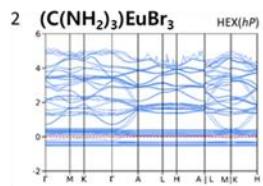
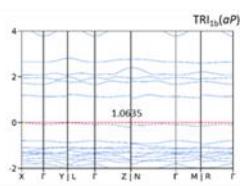
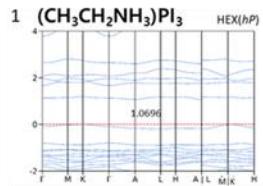
## NSAG-II 2<sup>nd</sup> Generation

Original symmetry setting

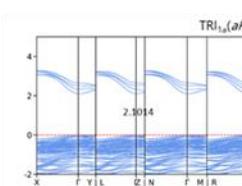
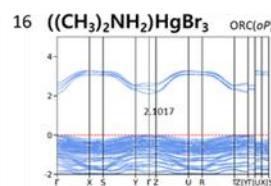
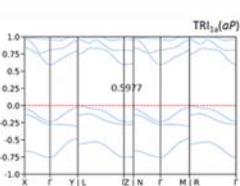
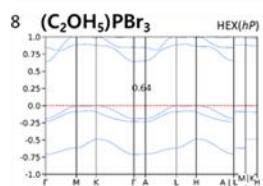
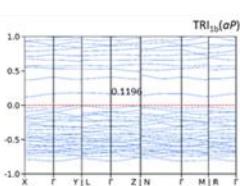
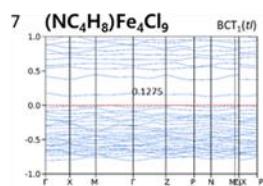
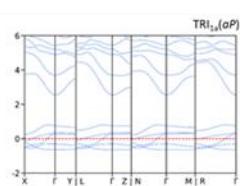
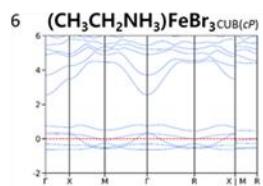
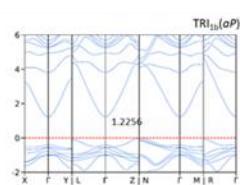
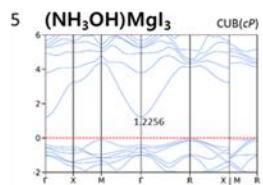
*P1* setting

Original symmetry setting

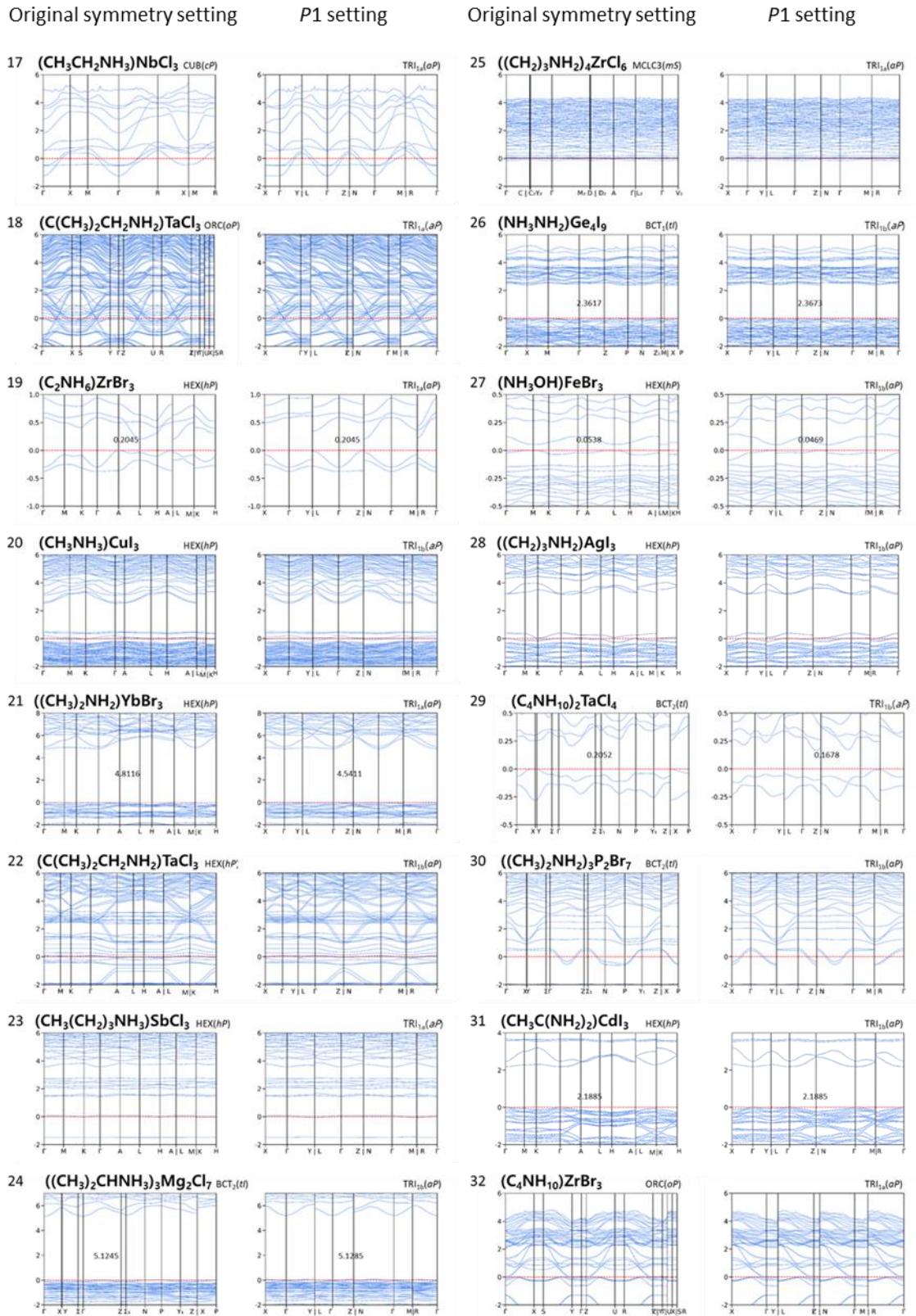
*P1* setting



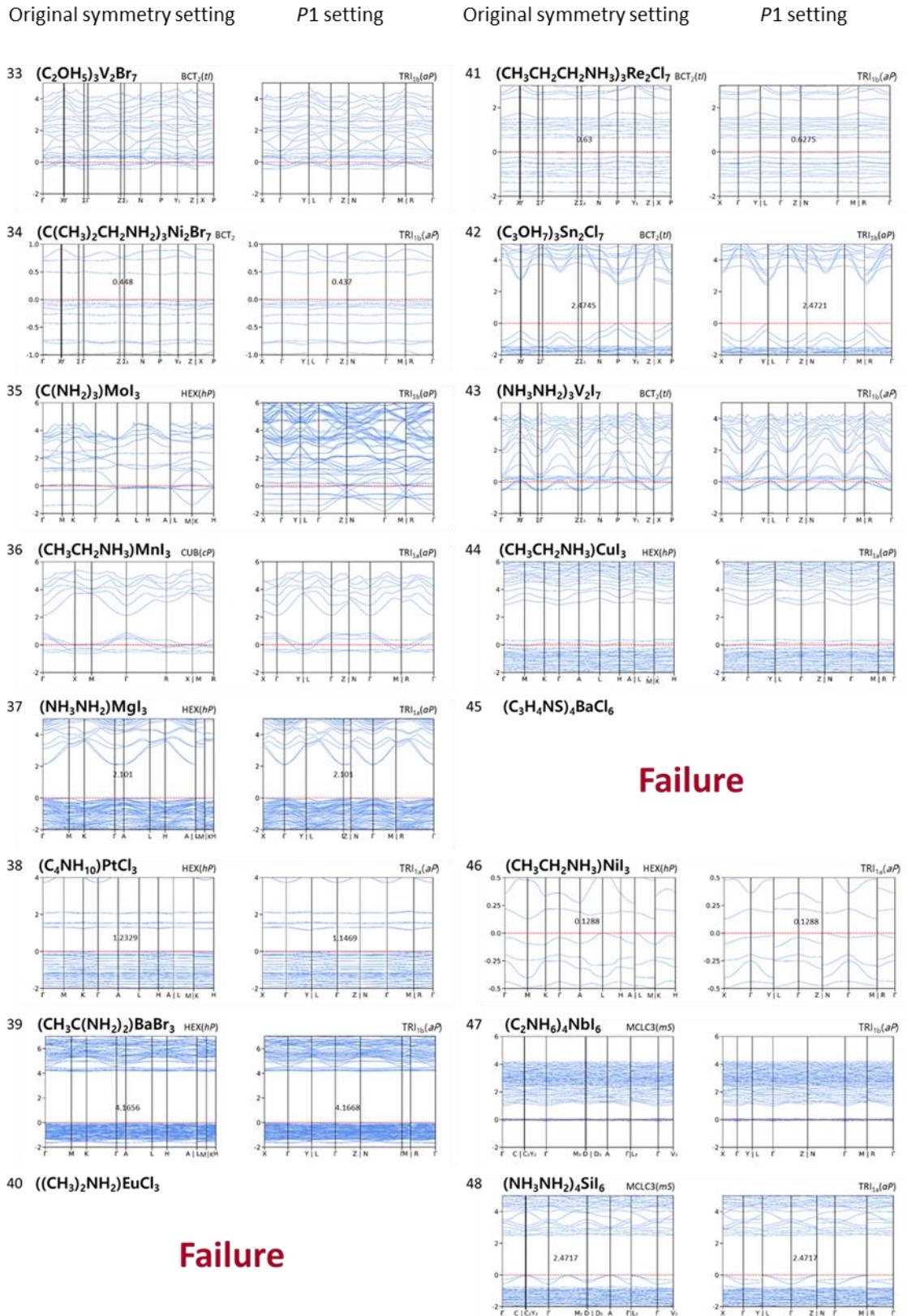
Failure



## NSAG-II 2<sup>nd</sup> Generation



## NSAG-II 2<sup>nd</sup> Generation



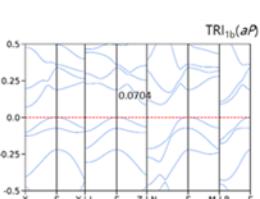
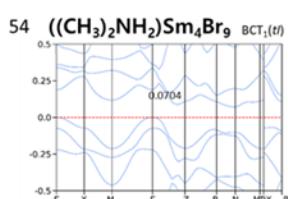
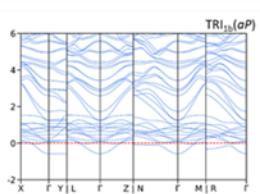
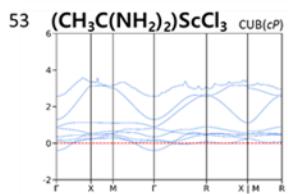
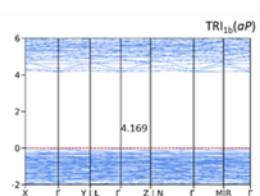
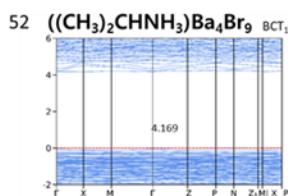
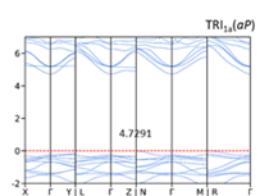
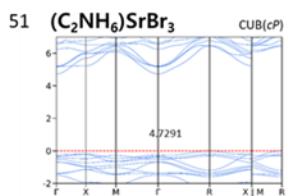
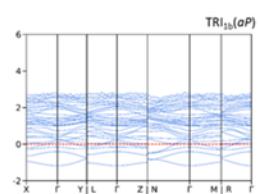
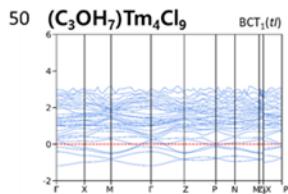
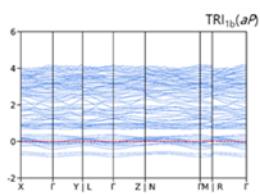
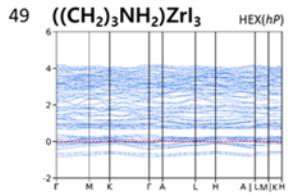
## NSAG-II 2<sup>nd</sup> Generation

Original symmetry setting

*P1* setting

Original symmetry setting

*P1* setting



## NSAG-II 3<sup>rd</sup> Generation

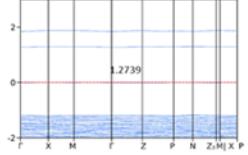
Original symmetry setting

*P1* setting

Original symmetry setting

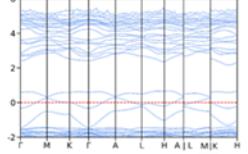
*P1* setting

1  $(C(CH_3)_2CH_2NH_2)Yb_4Cl_9$  BCT<sub>1</sub>(*t*)



TRI<sub>1b</sub>(*aP*)

2  $(C_2NH_6)InI_3$  HEX(*hP*)

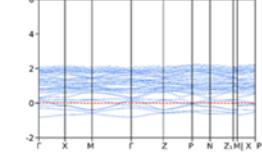


TRI<sub>1a</sub>(*aP*)

3  $((CH_3)_2CHNH_3)_3NiI_7$

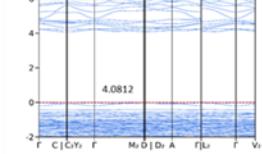
Failure

9  $((CH_3)_3NH)Y_4I_9$  BCT<sub>1</sub>(*t*)



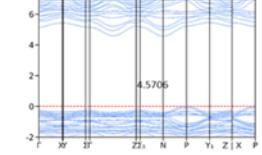
TRI<sub>1b</sub>(*aP*)

10  $(NH_3NH_2)_4GeCl_6$  MCLC3(*mS*)



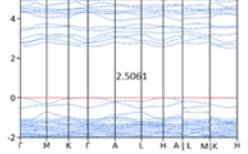
TRI<sub>1a</sub>(*aP*)

11  $(C_2OH_5)_3Yb_2Cl_7$  BCT<sub>2</sub>(*t*)



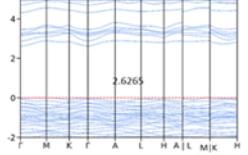
TRI<sub>1b</sub>(*aP*)

4  $(C(NH_2)_3)SnBr_3$  HEX(*hP*)



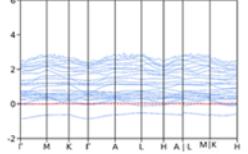
TRI<sub>1a</sub>(*aP*)

5  $(CH(NH_2)_2)ZnI_3$  HEX(*hP*)



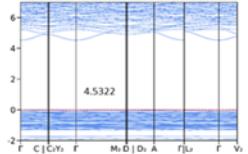
TRI<sub>1a</sub>(*aP*)

6  $(CH_3C(NH_2)_2)_2YI_3$  HEX(*hP*)



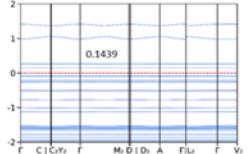
TRI<sub>1a</sub>(*aP*)

7  $((CH_3)_2NH_2)_4YbBr_6$  MCLC3(*mS*)



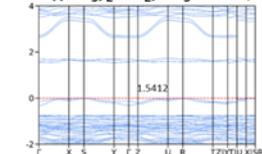
TRI<sub>1a</sub>(*aP*)

8  $(C_2OH_5)_4CoI_6$  MCLC3(*mS*)



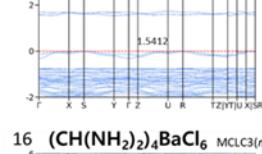
TRI<sub>1a</sub>(*aP*)

12  $((CH_3)_2NH_2)_3Sb_2Cl_7$  BCT<sub>2</sub>(*t*)



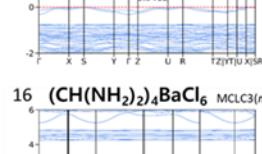
TRI<sub>1b</sub>(*aP*)

13  $((CH_3)_2NH_2)_4VBr_6$  MCLC3(*mS*)



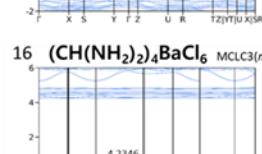
TRI<sub>1a</sub>(*aP*)

14  $(CH_3C(NH_2)_2)_4CaBr_6$  MCLC3(*mS*)



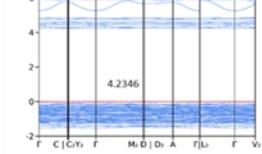
TRI<sub>1a</sub>(*aP*)

15  $((CH_3)_2NH_2)_3InI_3$  ORC(*oP*)



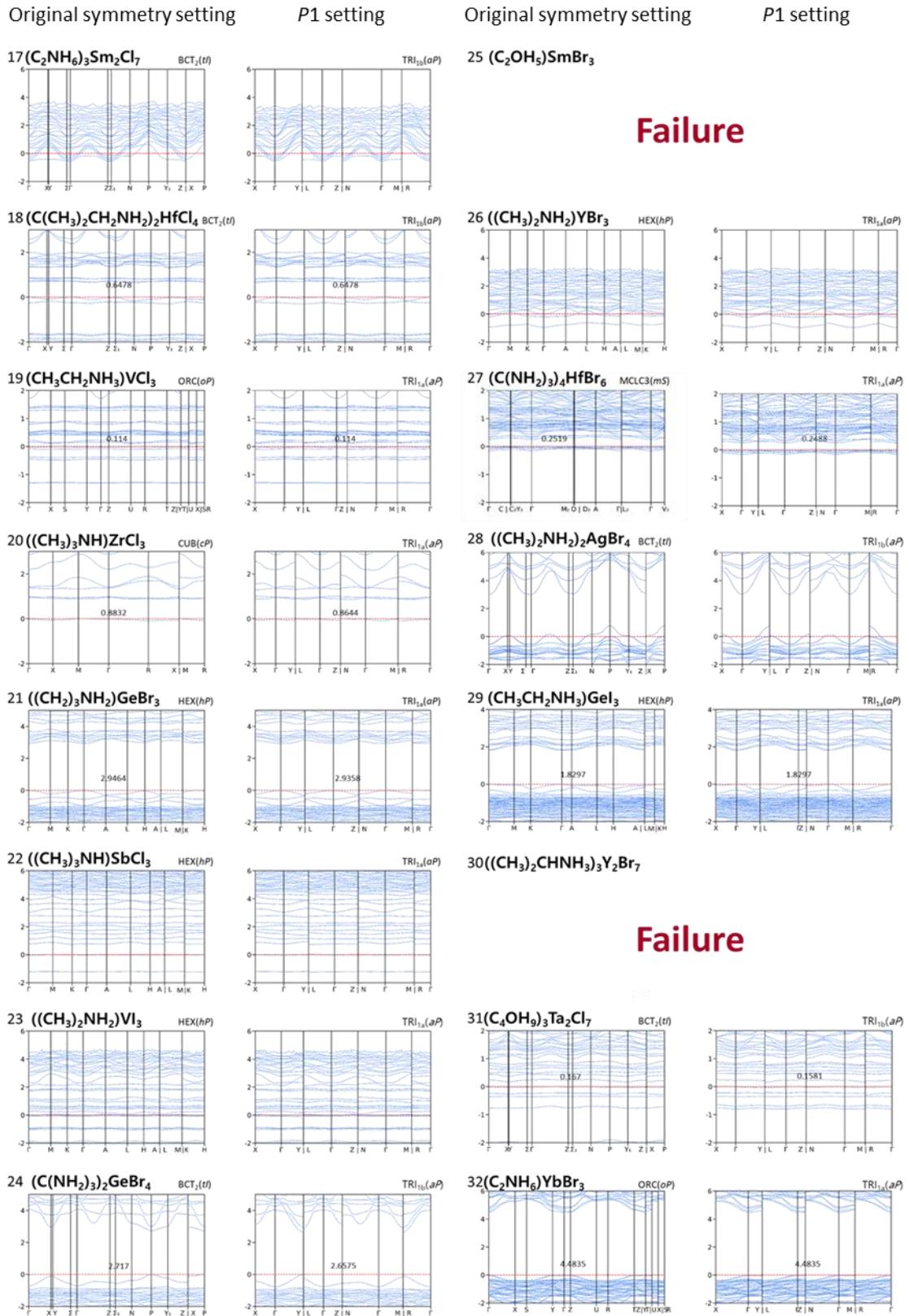
TRI<sub>1b</sub>(*aP*)

16  $(CH(NH_2)_2)_4BaCl_6$  MCLC3(*mS*)

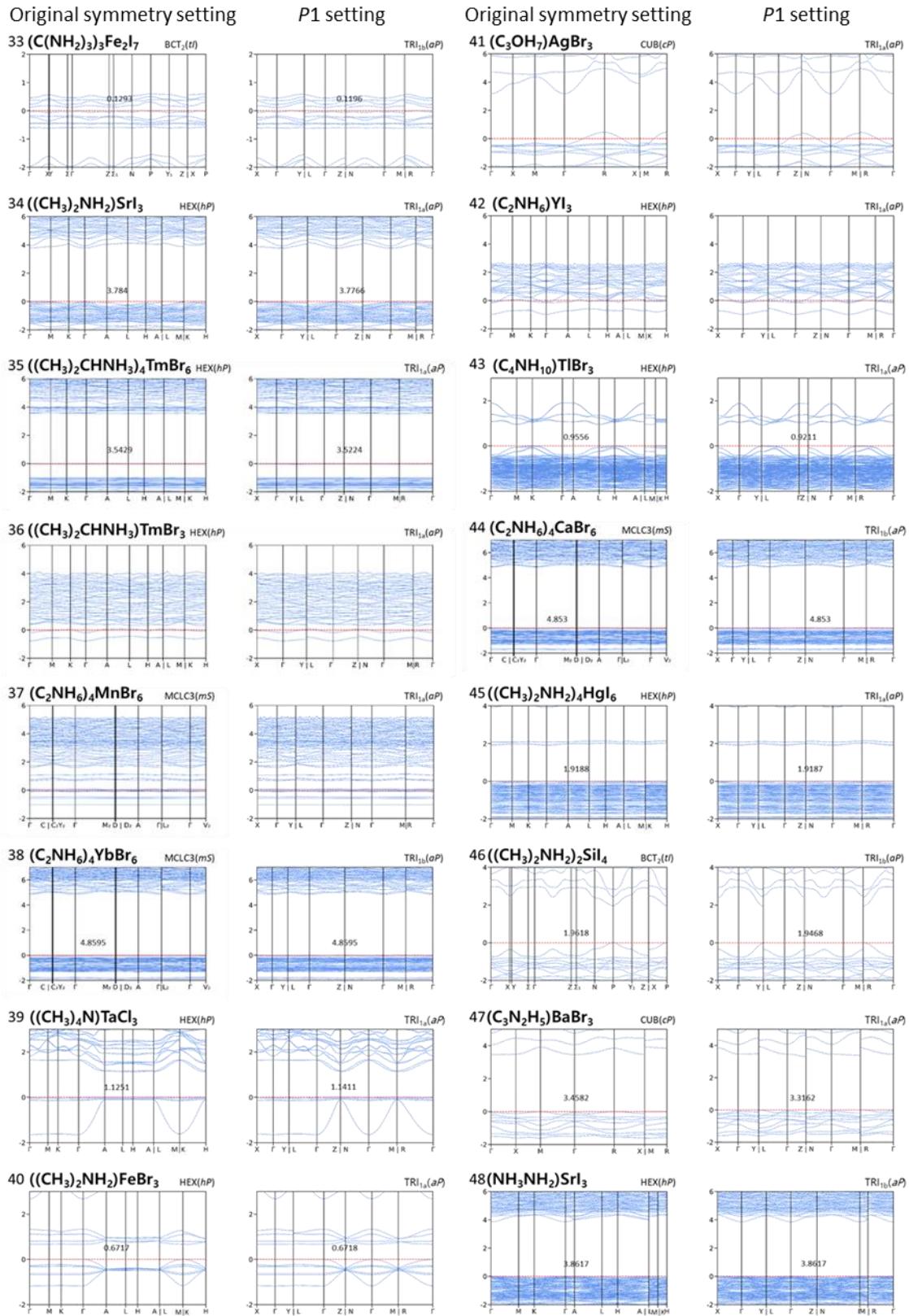


TRI<sub>1b</sub>(*aP*)

## NSAG-II 3<sup>rd</sup> Generation

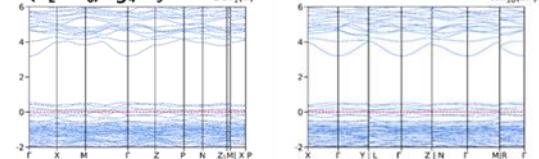
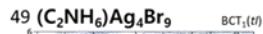


## NSAG-II 3<sup>rd</sup> Generation

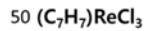


## NSAG-II 3<sup>rd</sup> Generation

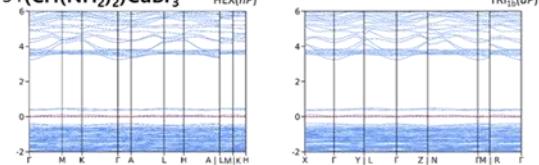
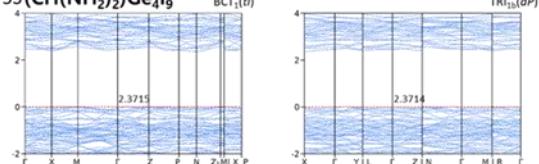
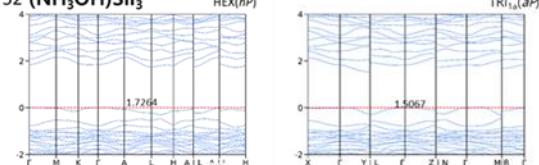
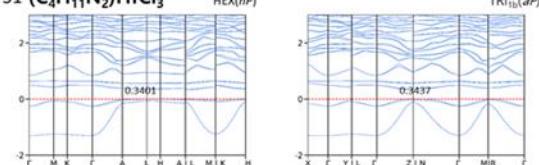
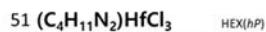
Original symmetry setting



$P1$  setting

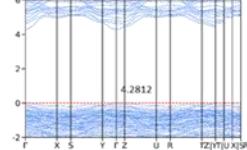
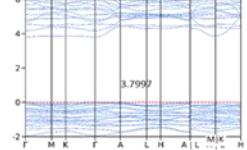
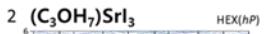
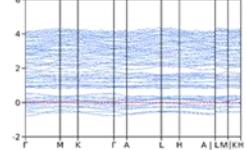
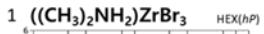


## Failure

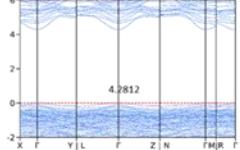
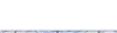
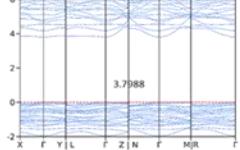
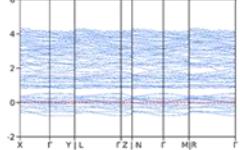


## NSAG-II 4<sup>th</sup> Generation

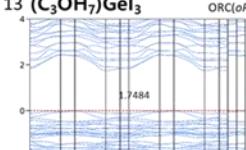
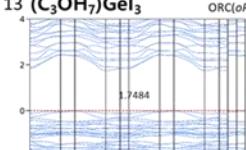
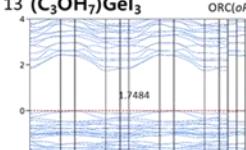
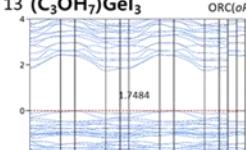
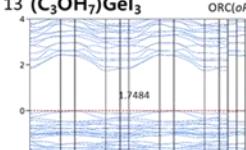
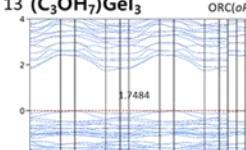
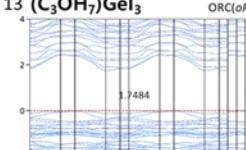
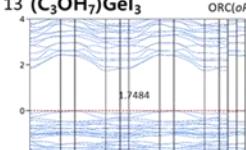
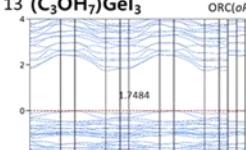
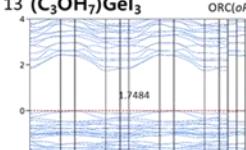
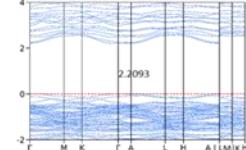
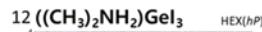
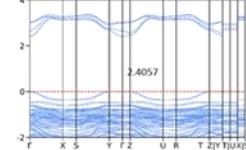
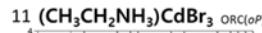
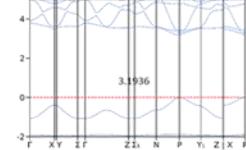
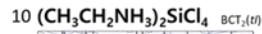
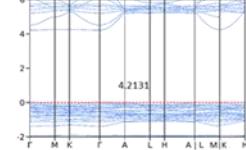
Original symmetry setting



*P1* setting



Original symmetry setting

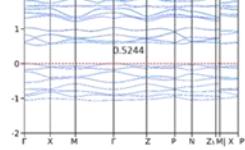


Failure

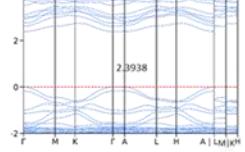
## NSAG-II 4<sup>th</sup> Generation

Original symmetry setting

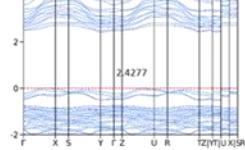
17  $((\text{CH}_3)_2\text{NH}_2)\text{Hf}_4\text{Br}_9$  BCT<sub>1</sub>(t)



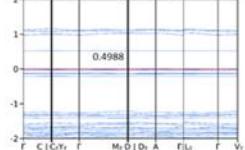
18  $(\text{NH}_3\text{OH})\text{GeCl}_3$  HEX(hP)



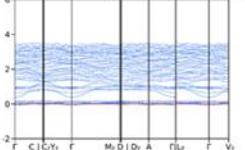
19  $((\text{CH}_3)_2\text{NH}_2)\text{SiI}_3$  ORC(oP)



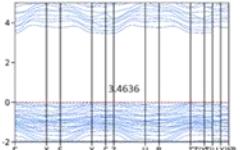
20  $((\text{CH}_2)_3\text{NH}_2)_4\text{FeI}_6$  MCLC3(mS)



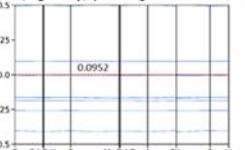
21  $(\text{NH}_3\text{NH}_2)_4\text{ScI}_6$  MCLC3(mS)



22  $(\text{CH}_3\text{NH}_3)\text{BeI}_3$  ORC(oP)



23  $(\text{C}_3\text{OH}_7)_4\text{NiBr}_6$  MCLC3(mS)



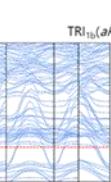
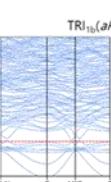
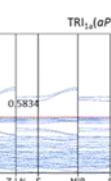
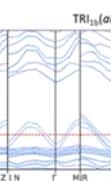
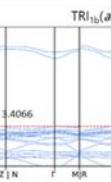
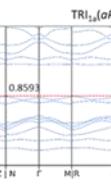
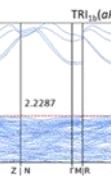
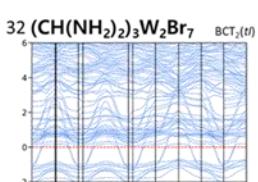
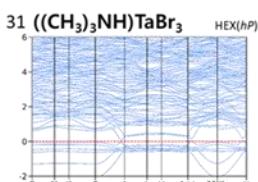
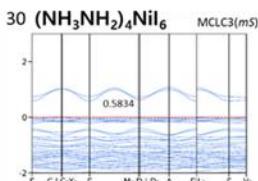
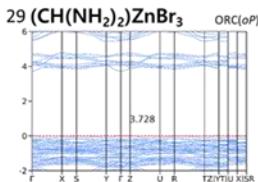
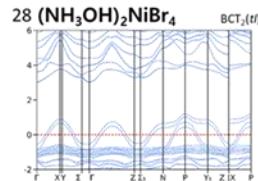
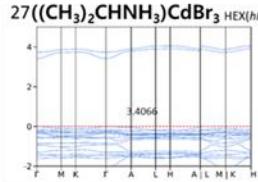
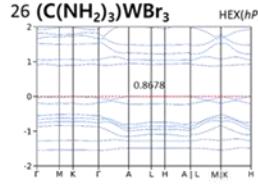
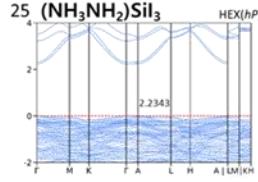
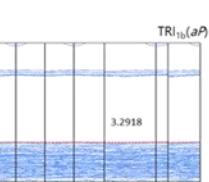
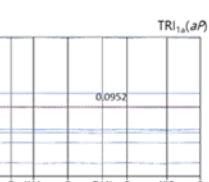
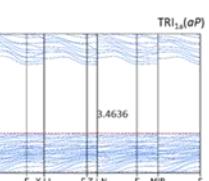
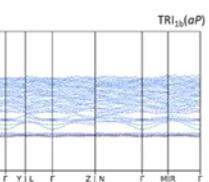
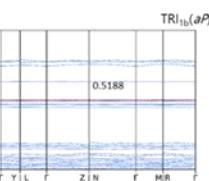
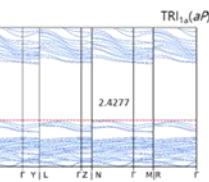
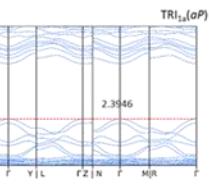
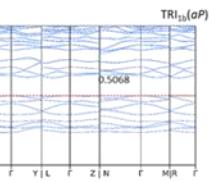
24  $(\text{NC}_4\text{H}_8)\text{YbCl}_3$  HEX(hP)



P1 setting

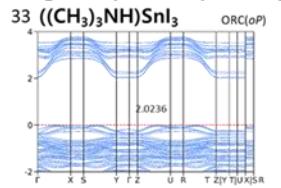
Original symmetry setting

P1 setting



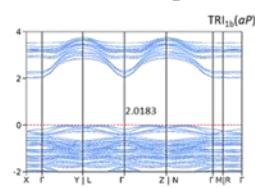
## NSAG-II 4<sup>th</sup> Generation

Original symmetry setting

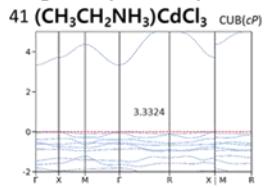


### Failure

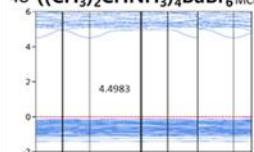
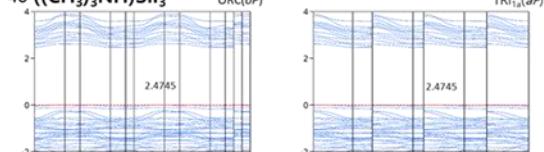
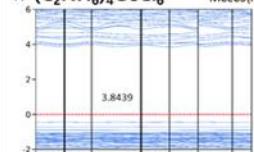
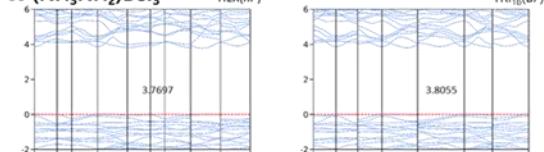
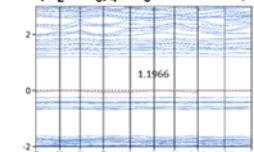
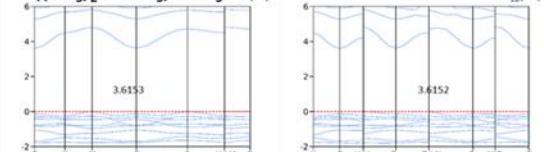
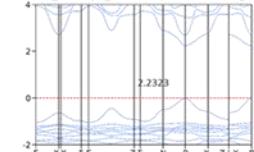
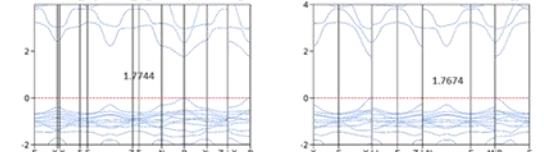
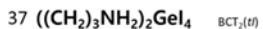
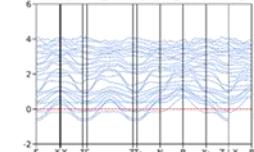
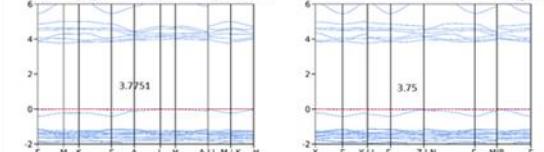
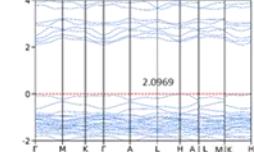
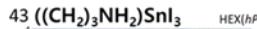
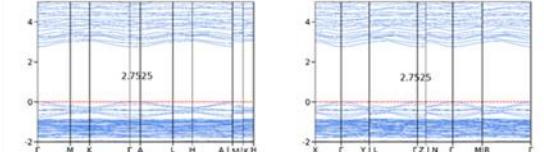
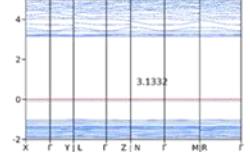
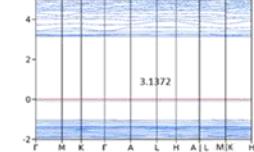
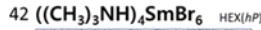
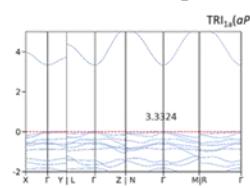
*P1* setting



Original symmetry setting

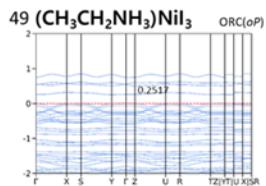


*P1* setting

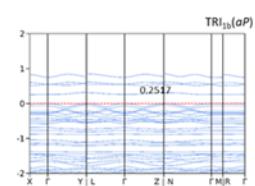


## NSAG-II 4<sup>th</sup> Generation

Original symmetry setting

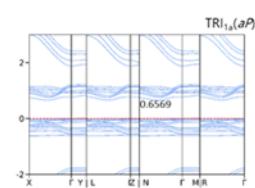
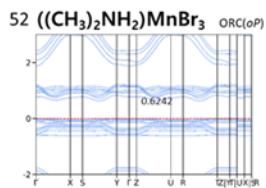
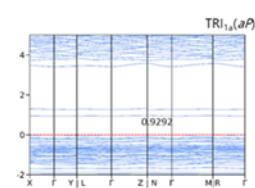
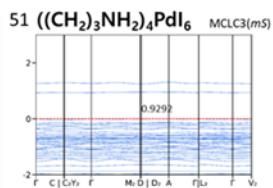
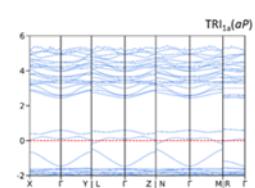
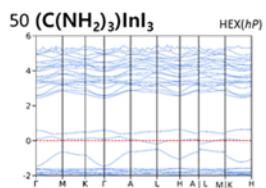


*P1* setting



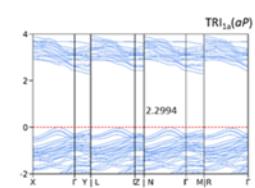
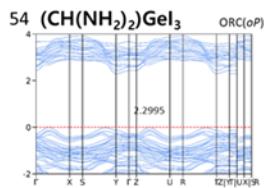
Original symmetry setting

*P1* setting

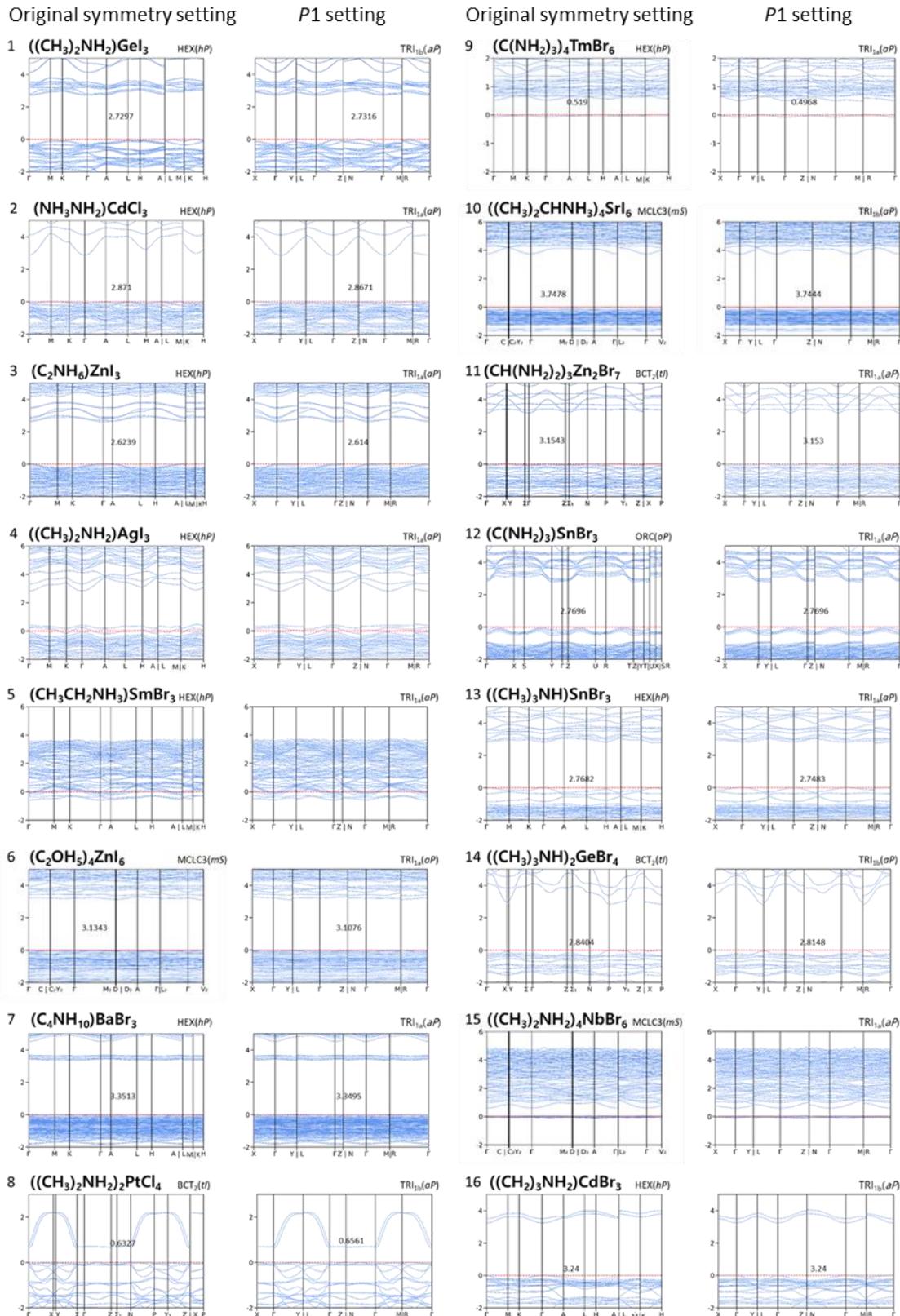


**53**  $(\text{C}(\text{NH}_2)_3)_4\text{AsBr}_6$

## Failure

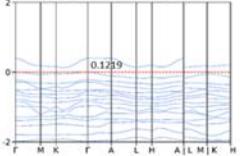
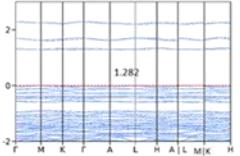
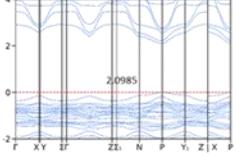
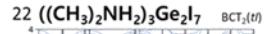
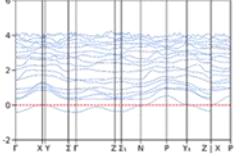
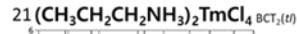
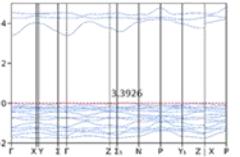
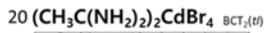
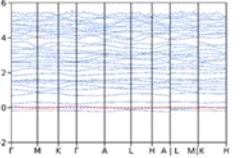
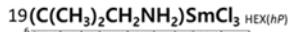
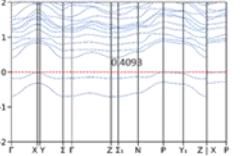
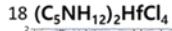
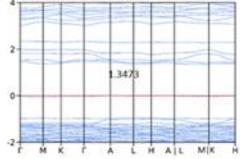
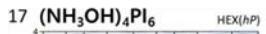


## NSAG-II 5<sup>th</sup> Generation

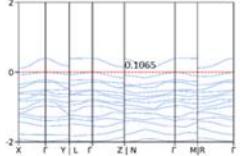
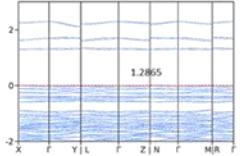
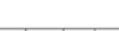
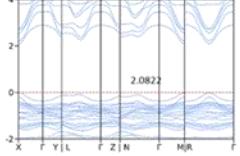
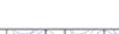
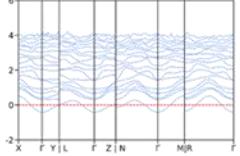
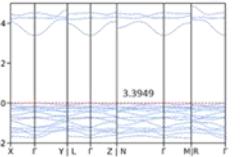
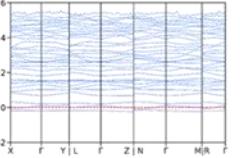
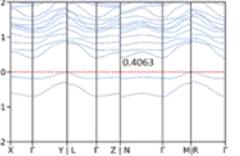
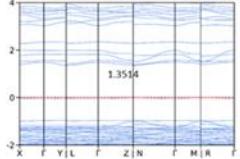


## NSAG-II 5<sup>th</sup> Generation

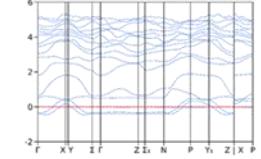
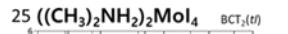
Original symmetry setting



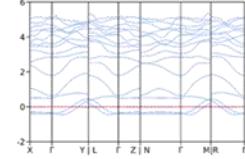
*P1* setting



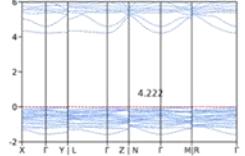
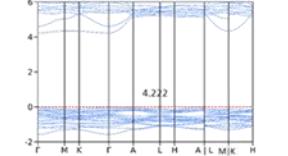
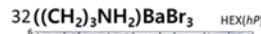
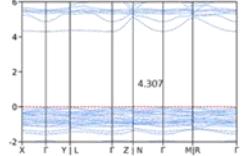
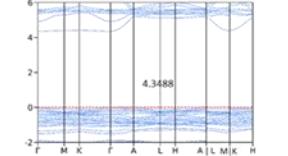
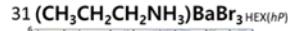
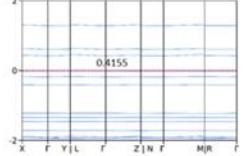
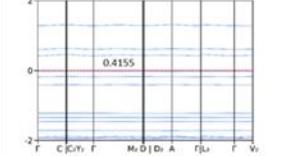
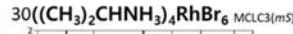
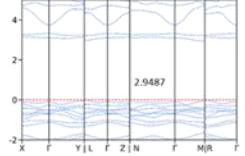
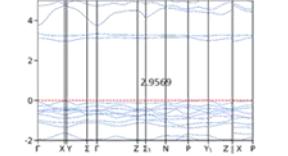
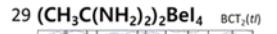
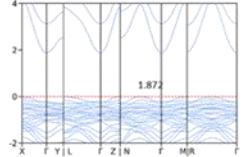
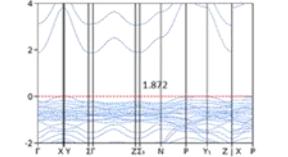
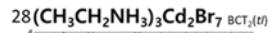
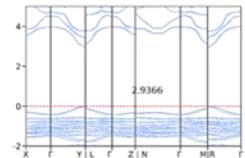
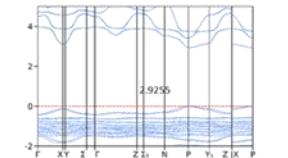
Original symmetry setting



*P1* setting

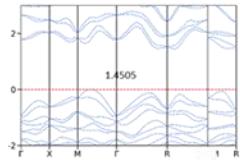
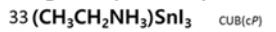


Failure



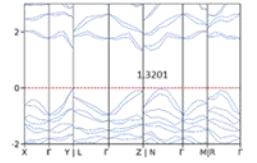
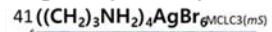
## NSAG-II 5<sup>th</sup> Generation

Original symmetry setting

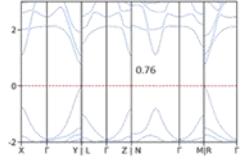
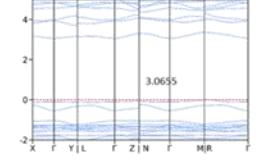
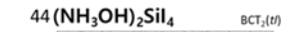
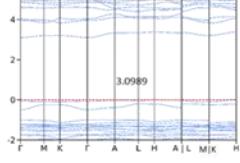
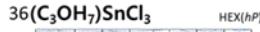
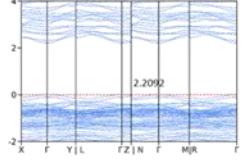
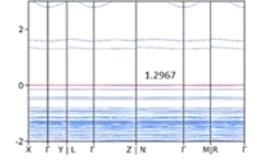
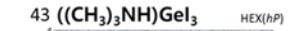
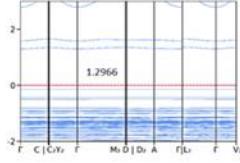
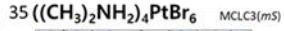
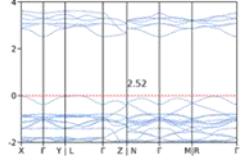
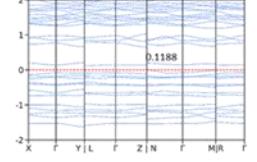
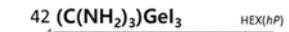
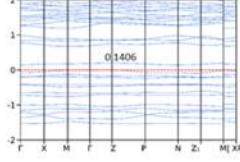
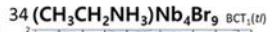
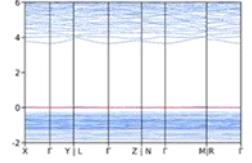


*P1* setting

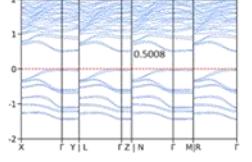
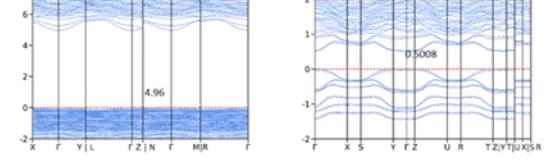
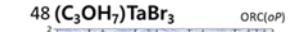
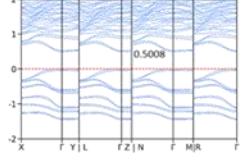
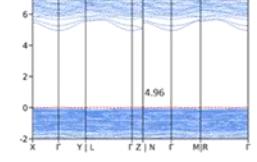
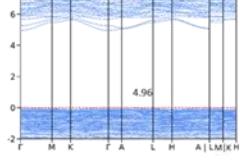
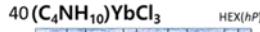
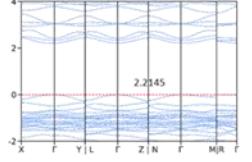
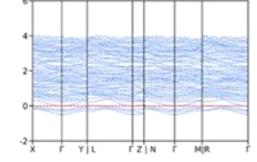
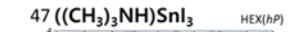
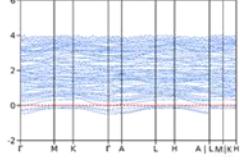
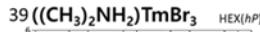
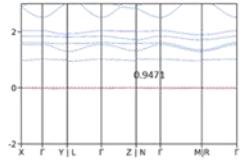
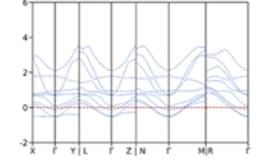
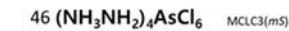
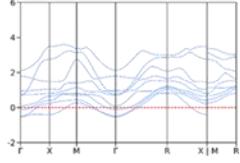
Original symmetry setting



*P1* setting

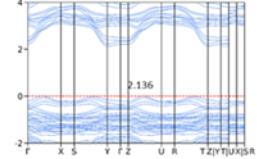
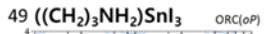


## Failure

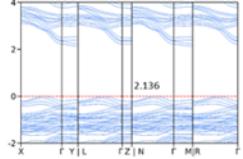


## NSAG-II 5<sup>th</sup> Generation

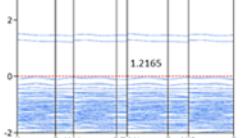
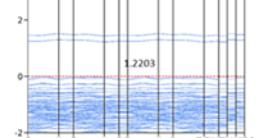
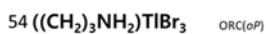
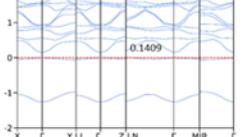
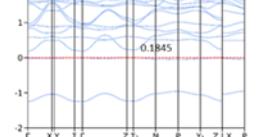
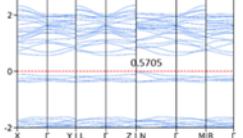
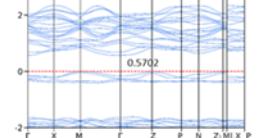
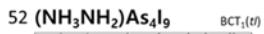
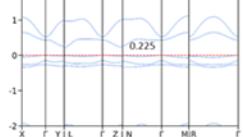
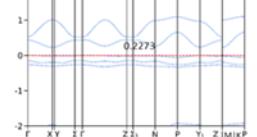
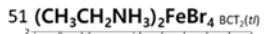
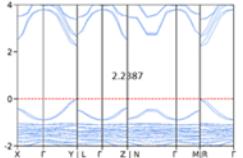
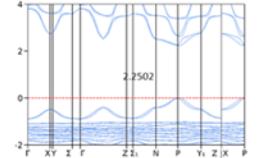
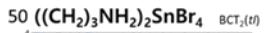
Original symmetry setting



*P*1 setting

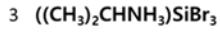
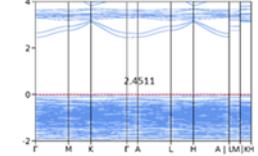
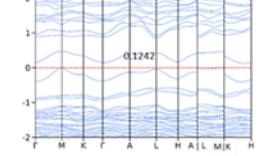


Original symmetry setting

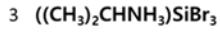
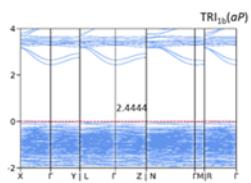
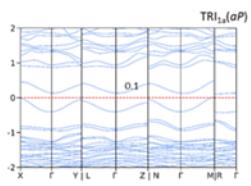


## NSAG-III 1<sup>st</sup> Generation

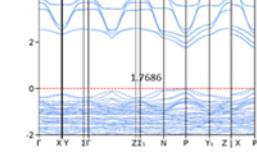
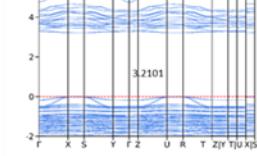
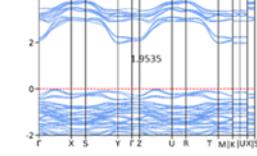
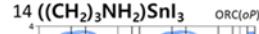
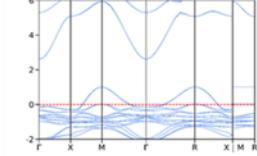
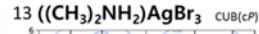
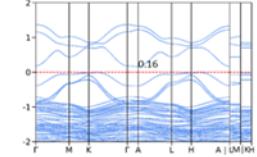
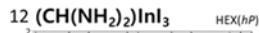
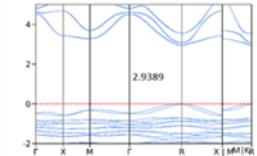
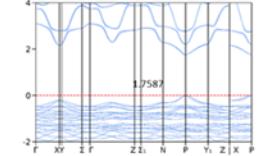
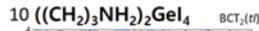
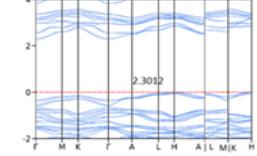
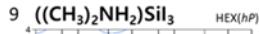
Original symmetry setting



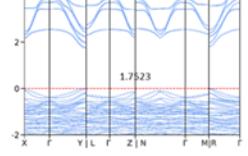
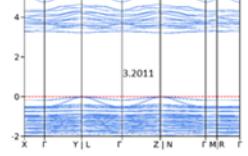
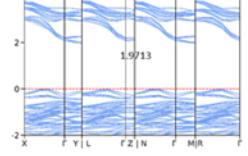
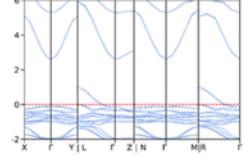
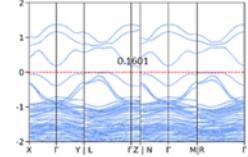
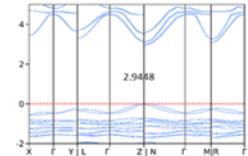
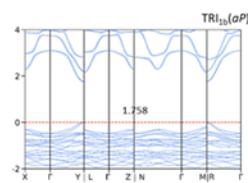
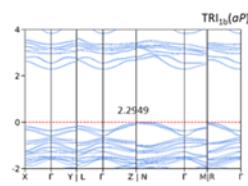
*P1* setting



Original symmetry setting



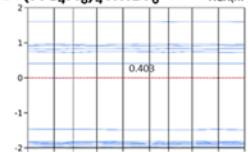
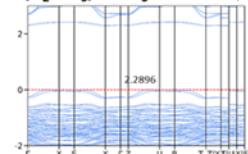
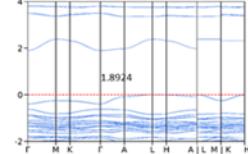
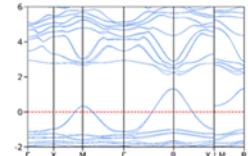
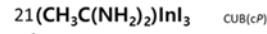
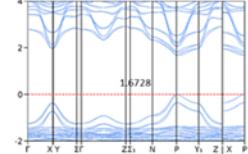
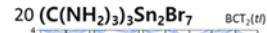
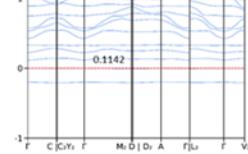
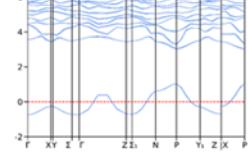
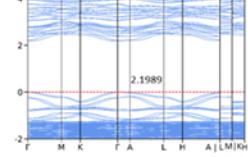
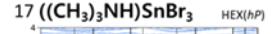
*P1* setting



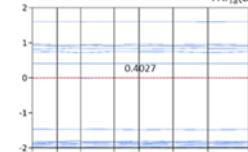
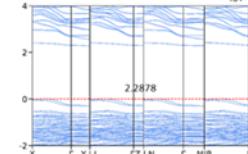
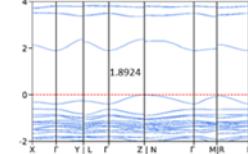
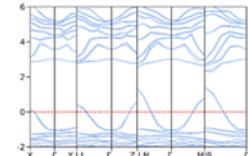
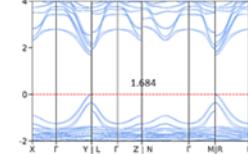
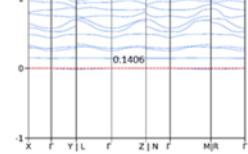
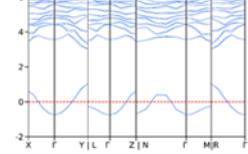
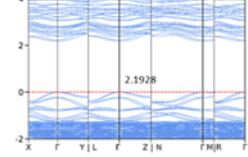
Failure

## NSAG-III 1<sup>st</sup> Generation

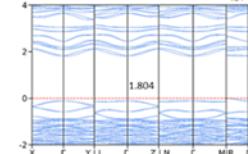
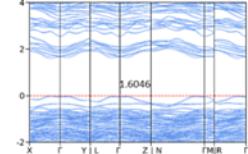
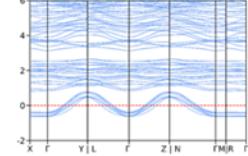
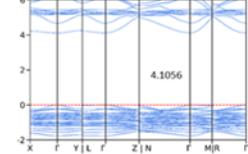
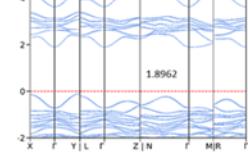
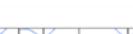
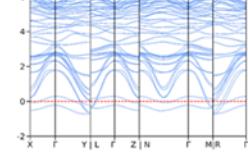
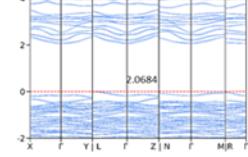
Original symmetry setting



*P1* setting



*P1* setting



## NSAG-III 1<sup>st</sup> Generation

Original symmetry setting

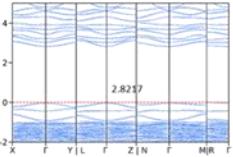
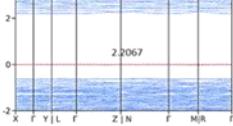
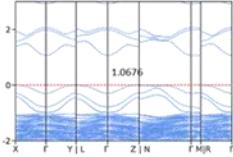
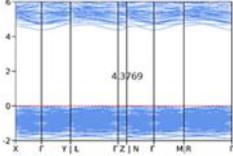
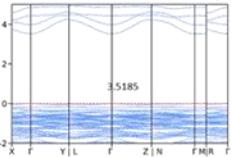
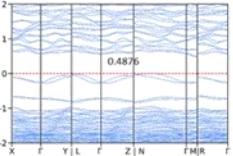
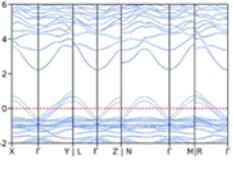
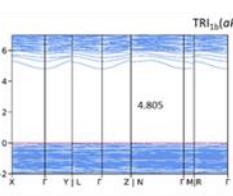
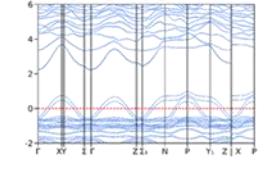
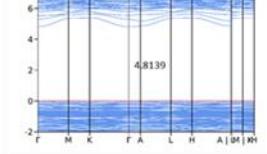
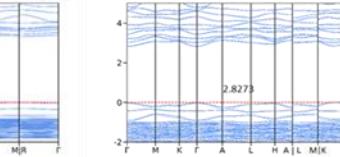
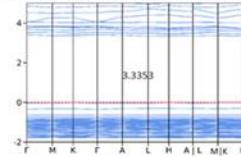
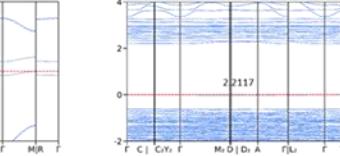
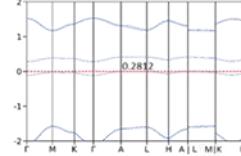
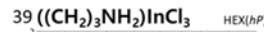
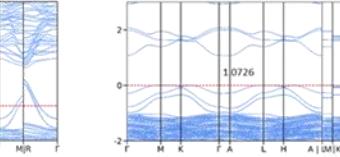
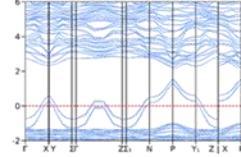
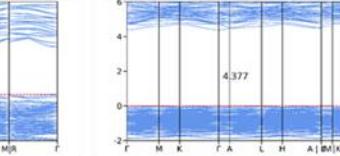
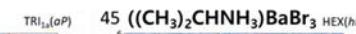
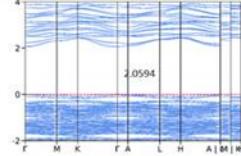
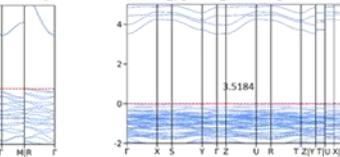
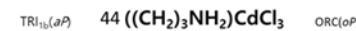
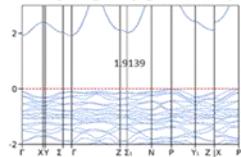
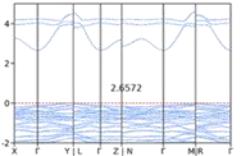
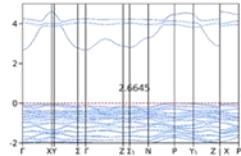
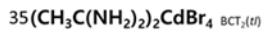
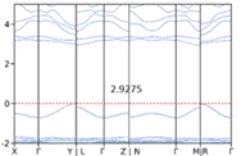
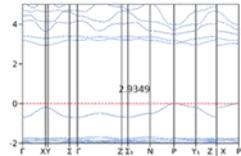
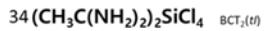


$P1$  setting

Original symmetry setting

$P1$  setting

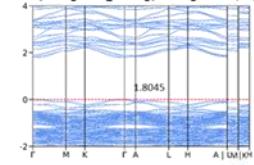
Failure



## NSAG-III 1<sup>st</sup> Generation

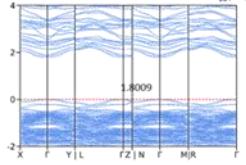
Original symmetry setting

49  $(\text{CH}_3\text{CH}_2\text{NH}_3)\text{GeI}_3$  HEX(*hP*)

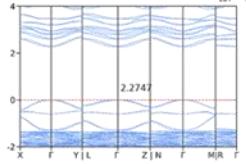
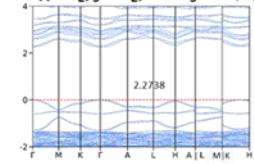


*P1* setting

TRI<sub>13</sub>(*aP*)

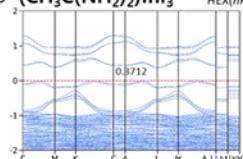
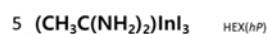
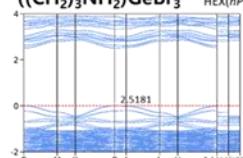
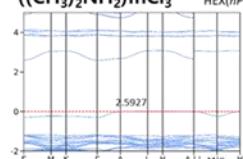
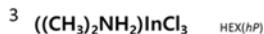
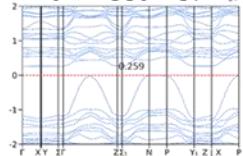
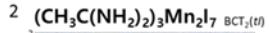
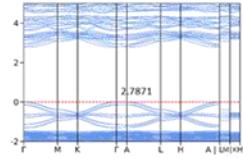
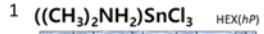


50  $((\text{CH}_2)_3\text{NH}_2)\text{SnBr}_3$  HEX(*hP*)



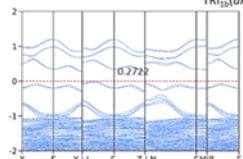
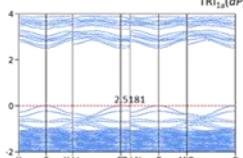
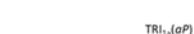
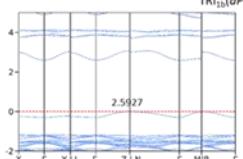
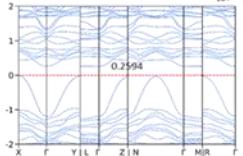
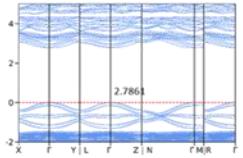
## NSAG-III 2<sup>nd</sup> Generation

Original symmetry setting



**Failure**

*P1* setting



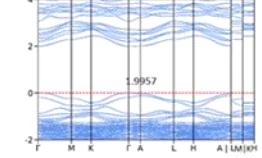
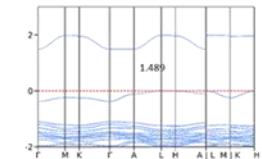
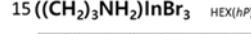
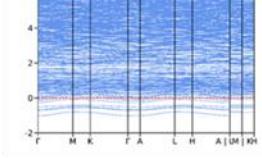
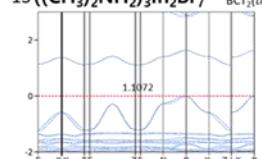
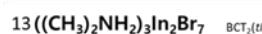
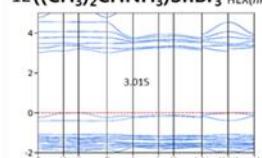
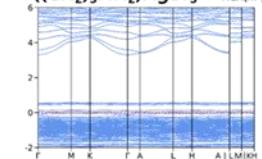
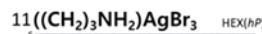
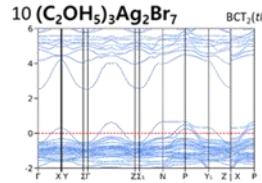
**Failure**

Original symmetry setting

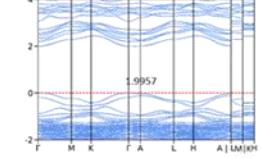
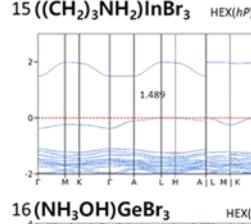
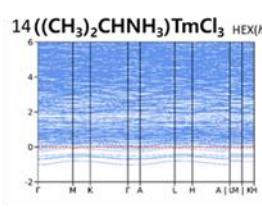
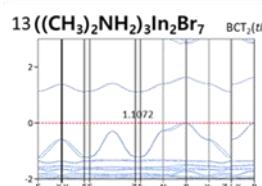
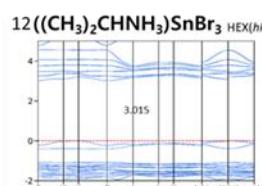
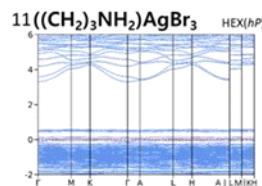
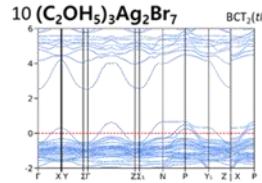


**Failure**

*P1* setting

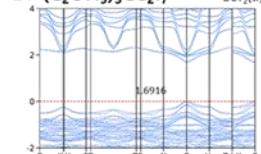
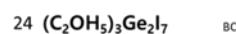
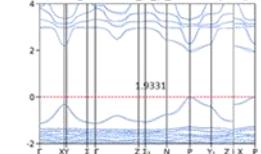
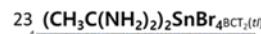
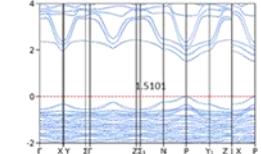
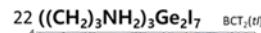
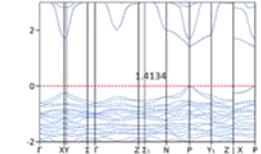
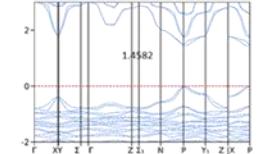
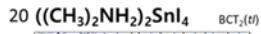
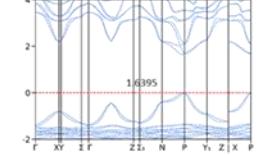
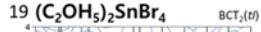
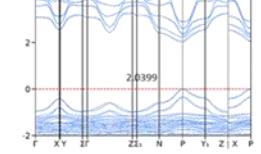
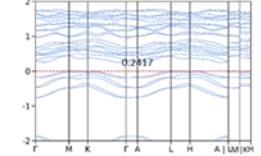


*P1* setting

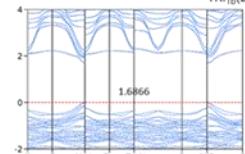
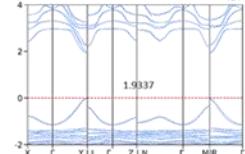
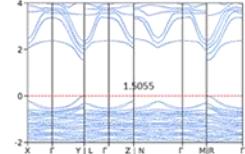
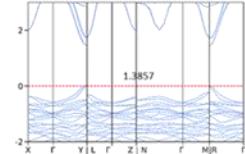
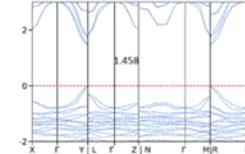
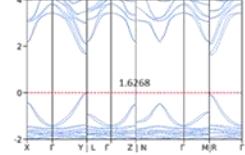
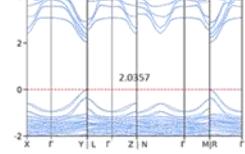
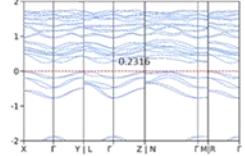


## NSAG-III 2<sup>nd</sup> Generation

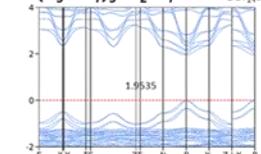
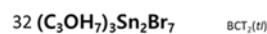
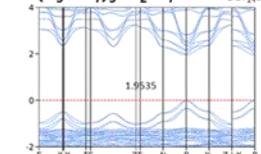
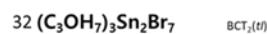
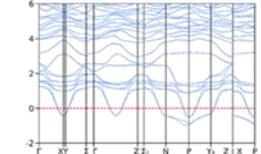
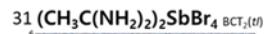
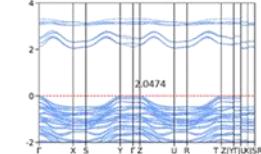
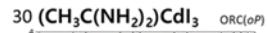
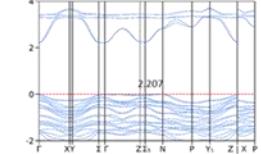
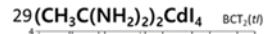
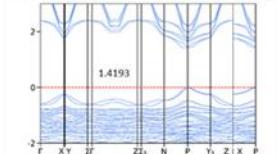
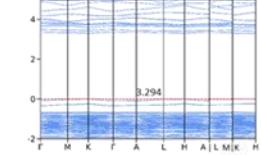
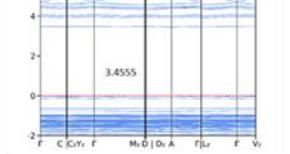
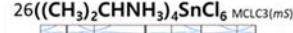
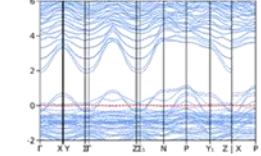
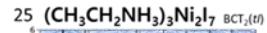
Original symmetry setting



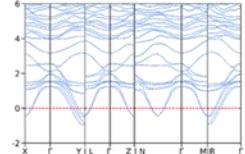
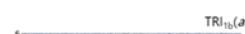
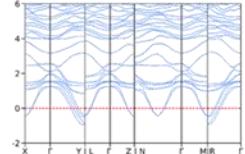
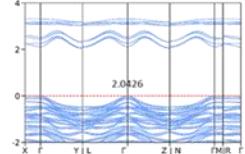
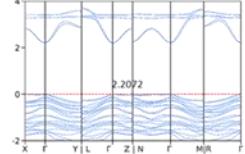
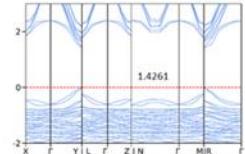
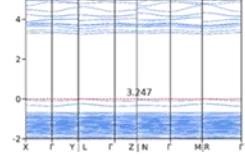
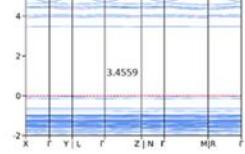
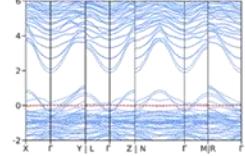
*P1* setting



Original symmetry setting

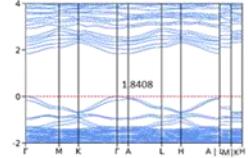


*P1* setting

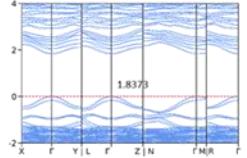


## NSAG-III 2<sup>nd</sup> Generation

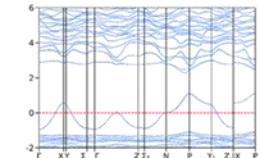
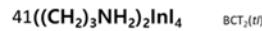
Original symmetry setting



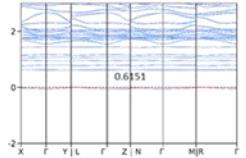
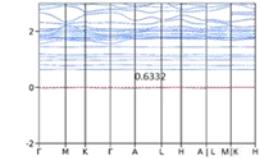
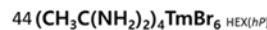
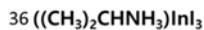
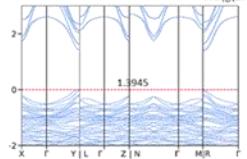
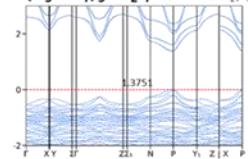
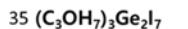
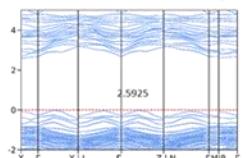
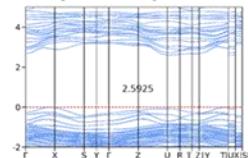
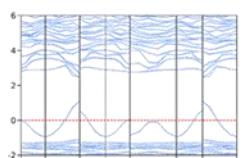
*P1* setting



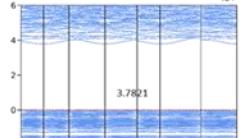
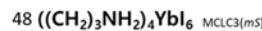
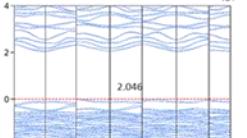
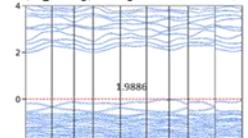
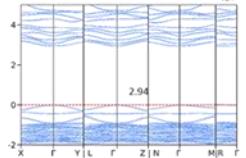
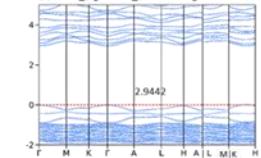
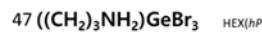
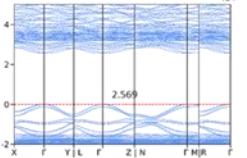
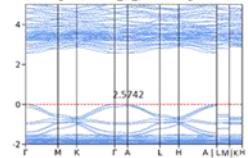
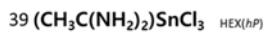
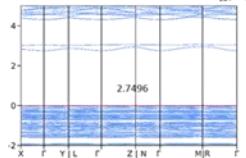
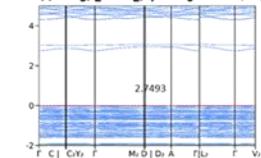
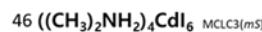
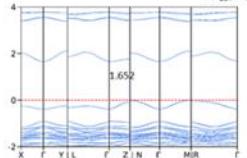
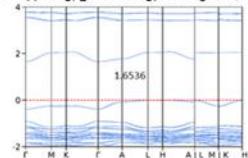
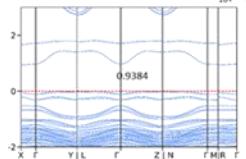
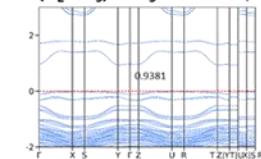
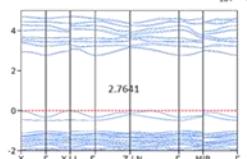
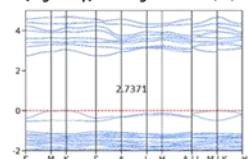
Original symmetry setting



*P1* setting



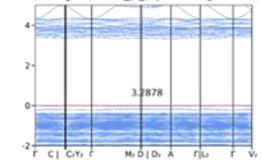
## Failure



## NSAG-III 2<sup>nd</sup> Generation

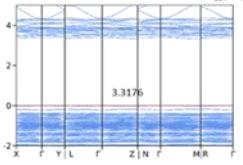
Original symmetry setting

49 ( $\text{CH}_3\text{C}(\text{NH}_2)_2\text{I}_4\text{GeBr}_6$ ) MCLC3(ms)

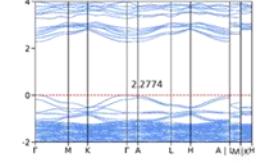


$P1$  setting

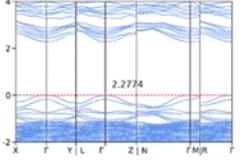
$\text{TRI}_{1a}(oP)$



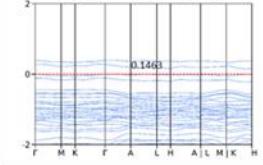
50 ( $\text{C}_2\text{NH}_6\text{GeBr}_3$ ) HEX(hP)



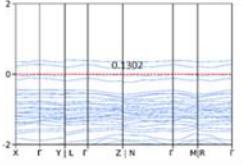
$\text{TRI}_{1b}(oP)$



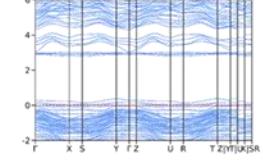
51 ( $(\text{CH}_3)_2\text{CHNH}_3\text{AgBr}_3$ ) HEX(hP)



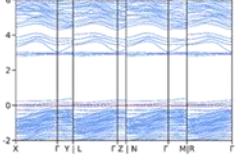
$\text{TRI}_{1b}(oP)$



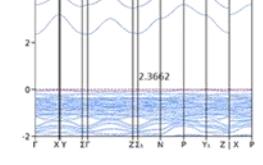
52 ( $\text{CH}_3\text{C}(\text{NH}_2)_2\text{AgI}_3$ ) ORC(oP)



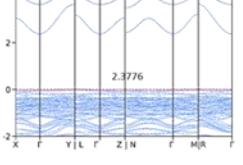
$\text{TRI}_{1a}(oP)$



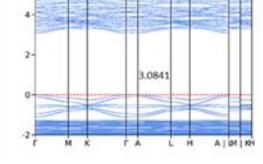
53 ( $(\text{CH}_2)_3\text{NH}_2)_3\text{Cd}_2\text{Br}_7$ ) BCT<sub>2</sub>(tf)



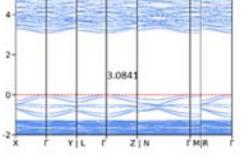
$\text{TRI}_{1b}(oP)$



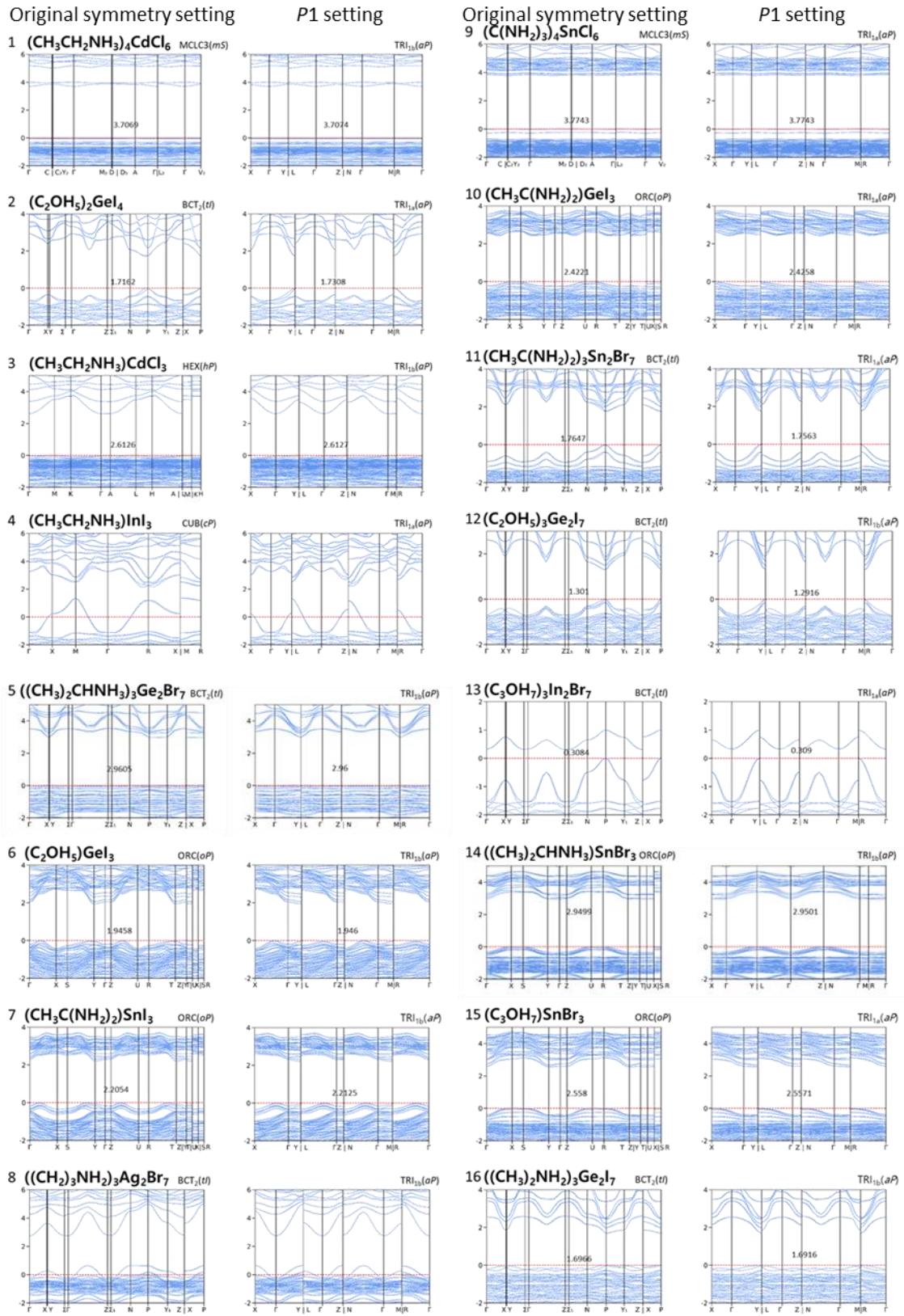
54 ( $(\text{CH}_3)_2\text{CHNH}_3\text{SnCl}_3$ ) HEX(hP)



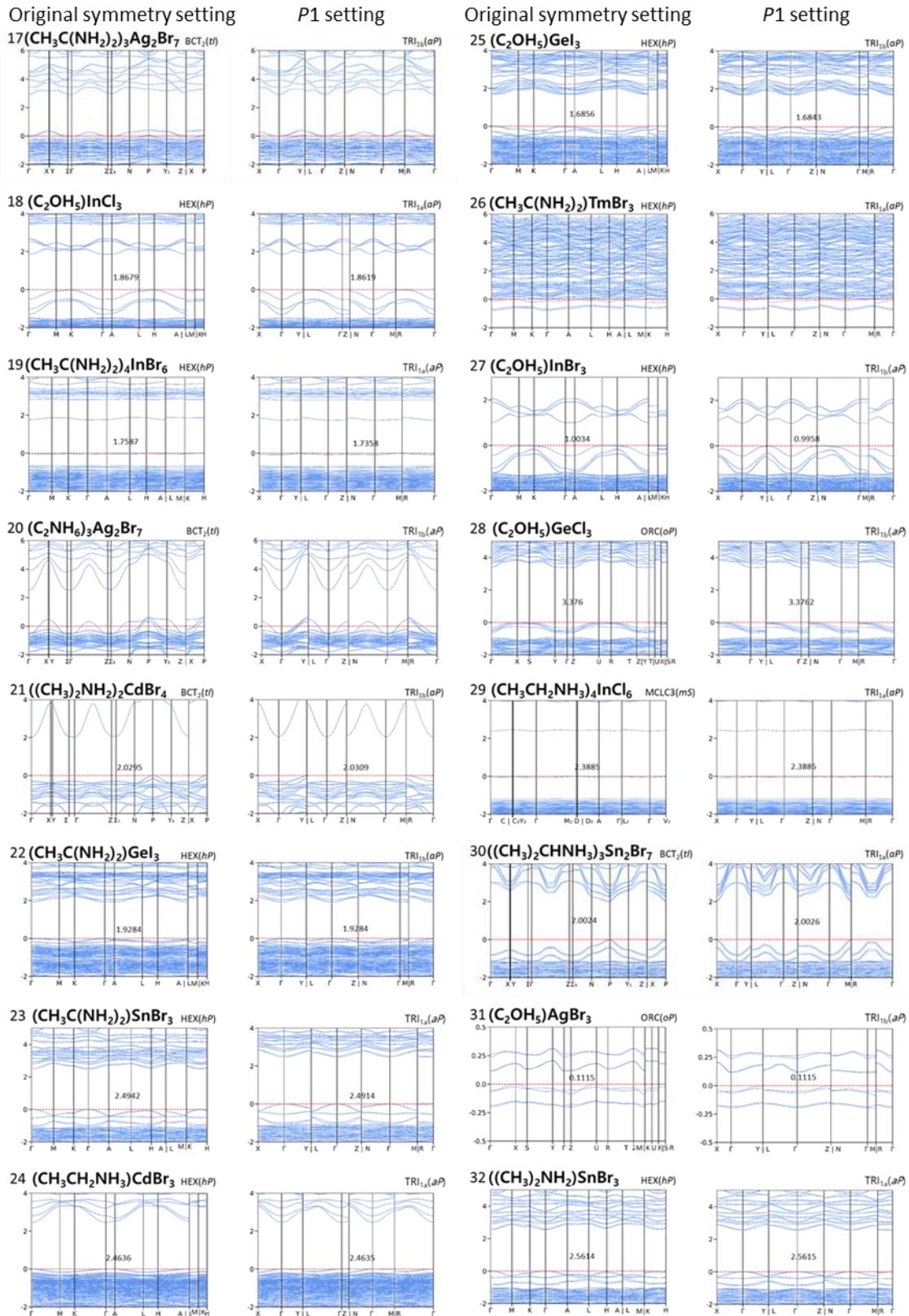
$\text{TRI}_{1b}(oP)$



## NSAG-III 3<sup>rd</sup> Generation

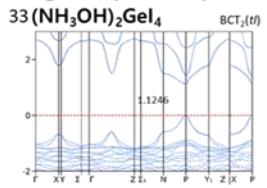


## NSAG-III 3<sup>rd</sup> Generation

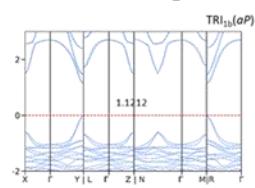


### NSAG-III 3<sup>rd</sup> Generation

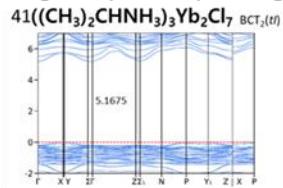
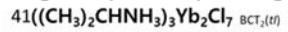
Original symmetry setting



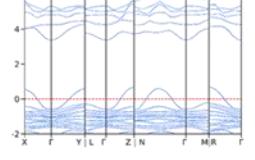
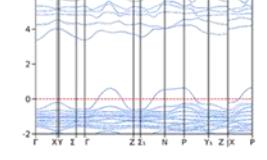
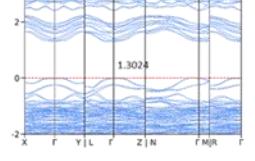
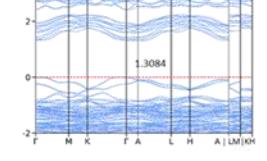
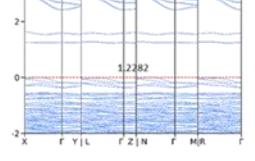
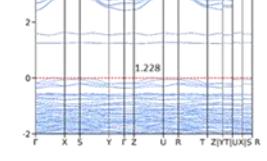
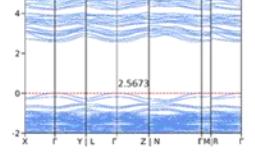
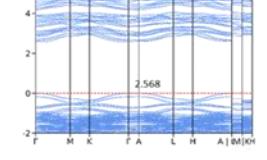
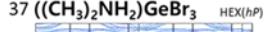
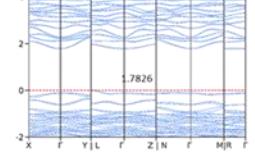
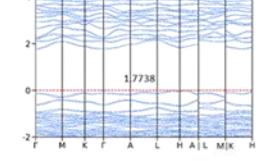
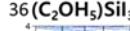
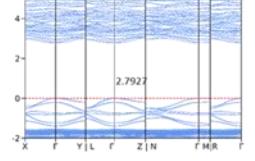
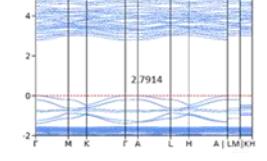
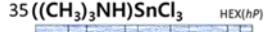
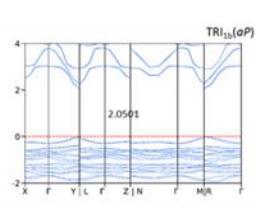
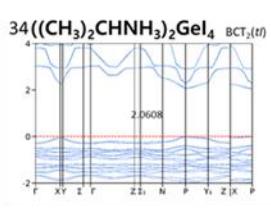
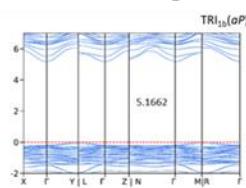
P1 setting



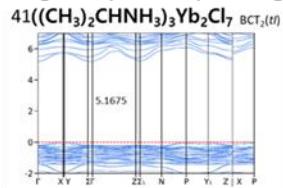
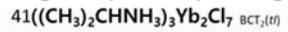
Original symmetry setting



P1 setting

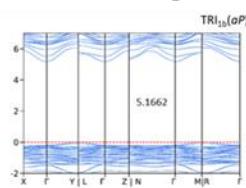


Original symmetry setting



P1 setting

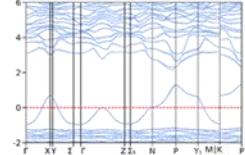
P1 setting



Failure

## NSAG-III 3<sup>rd</sup> Generation

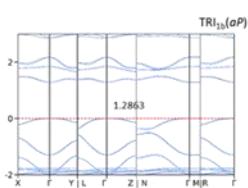
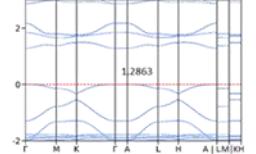
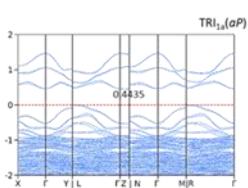
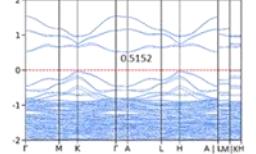
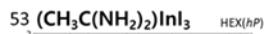
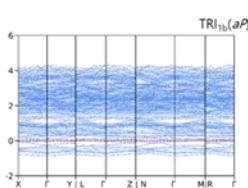
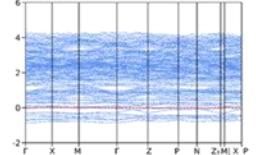
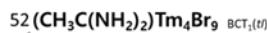
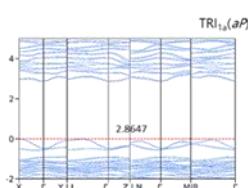
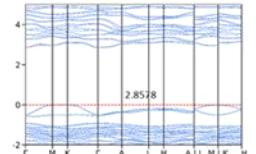
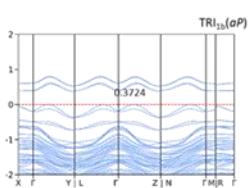
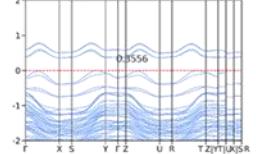
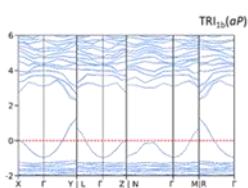
Original symmetry setting



*P1* setting

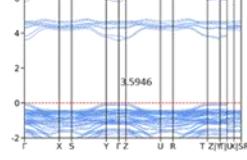
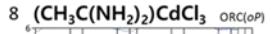
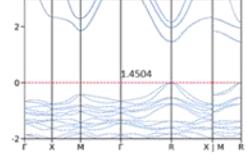
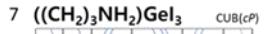
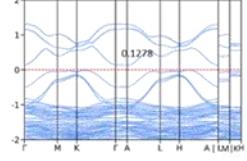
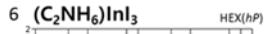
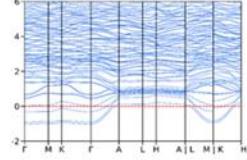
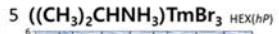
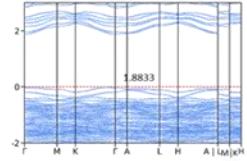
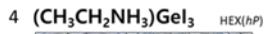
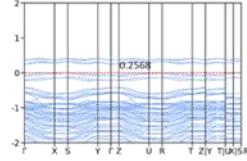
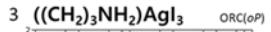
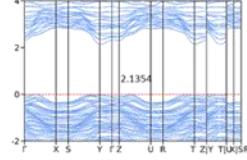
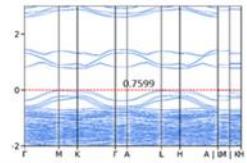
Original symmetry setting

*P1* setting

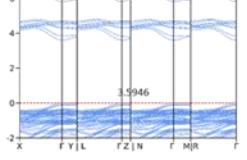
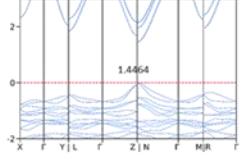
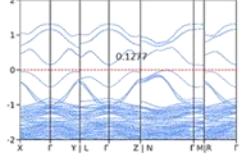
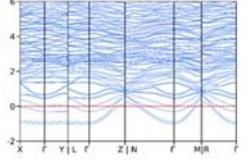
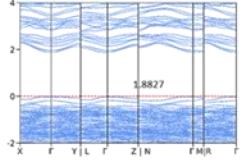
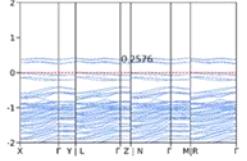
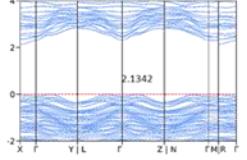
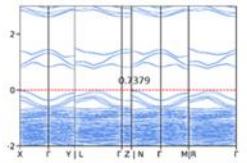


## NSAG-III 4<sup>th</sup> Generation

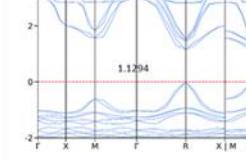
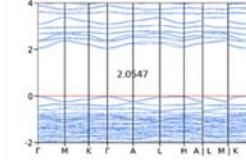
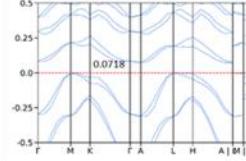
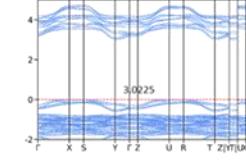
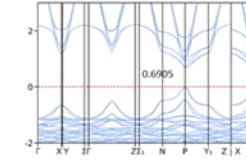
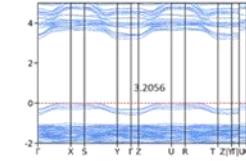
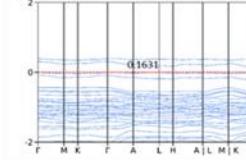
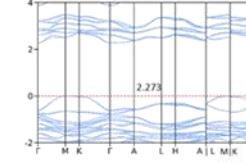
Original symmetry setting



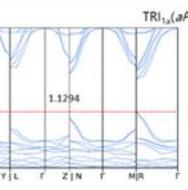
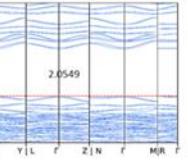
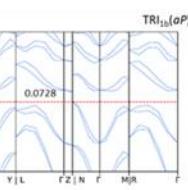
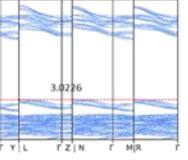
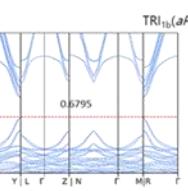
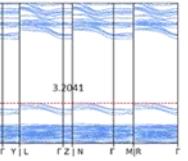
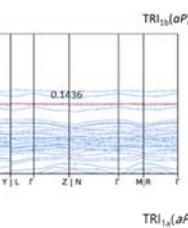
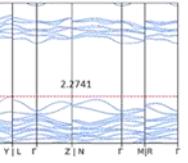
*P1* setting



Original symmetry setting

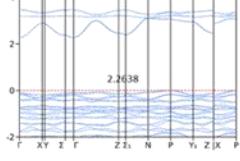
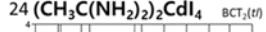
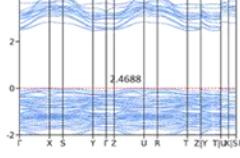
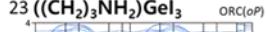
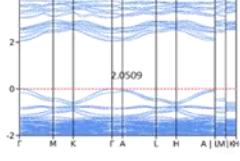
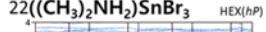
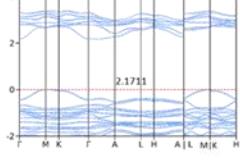
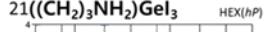
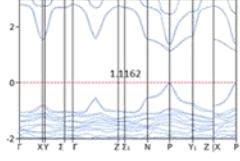
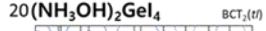
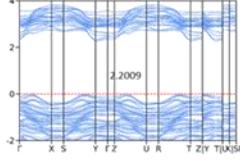
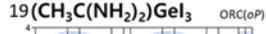
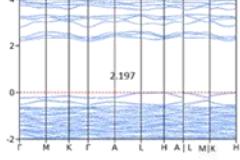
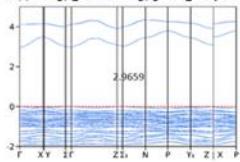


*P1* setting

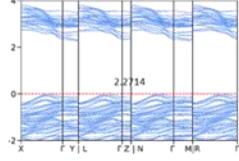
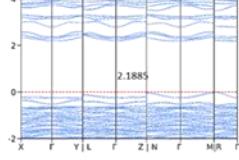
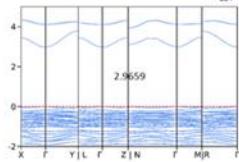


## NSAG-III 4<sup>th</sup> Generation

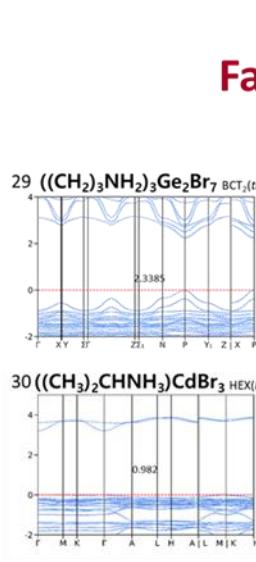
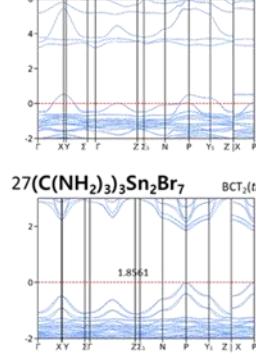
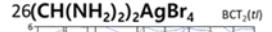
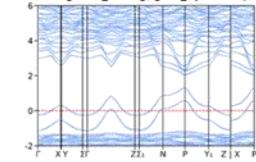
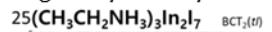
Original symmetry setting



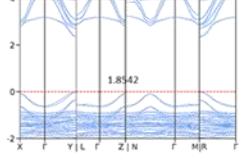
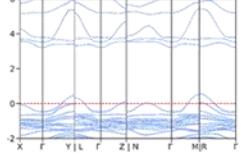
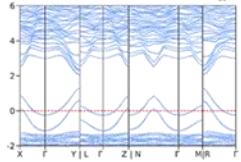
P1 setting



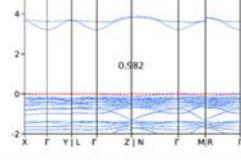
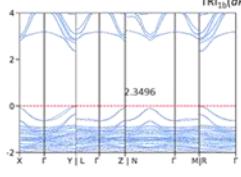
Original symmetry setting



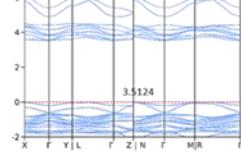
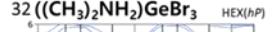
P1 setting



## Failure

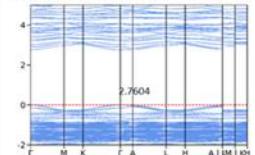
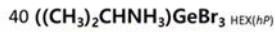
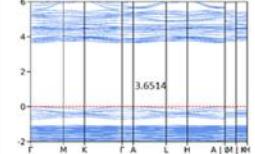
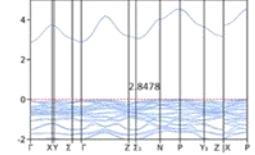
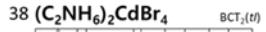
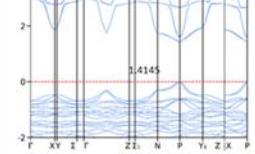
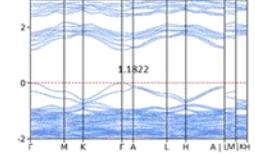
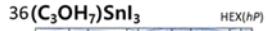
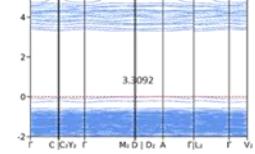
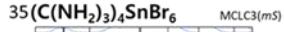
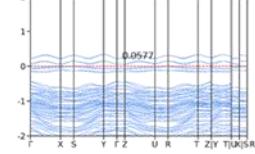
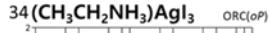
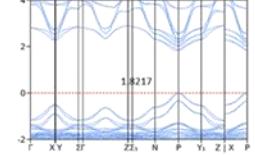
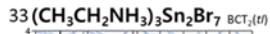


## Failure

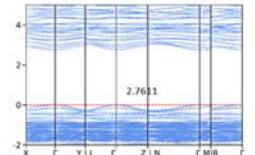
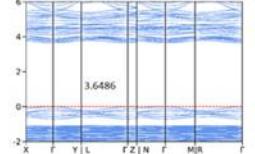
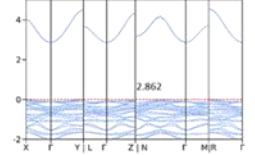
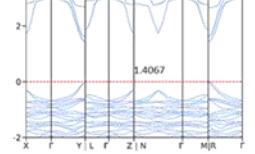
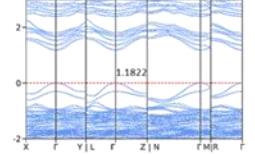
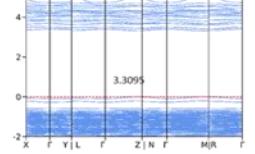
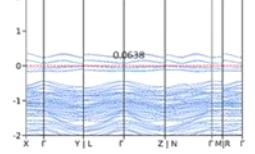
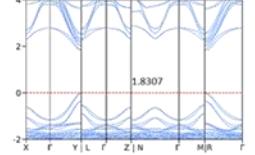


## NSAG-III 4<sup>th</sup> Generation

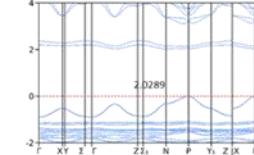
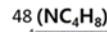
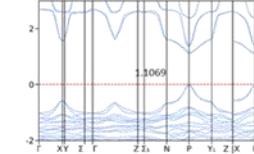
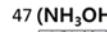
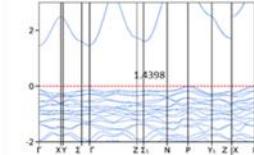
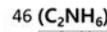
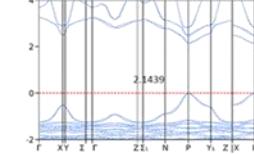
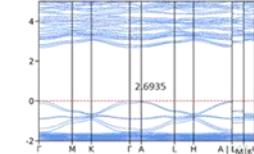
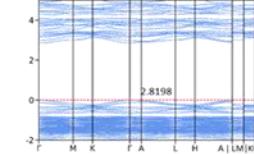
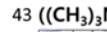
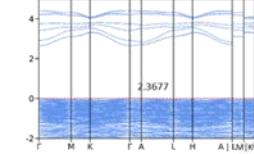
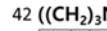
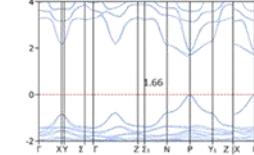
Original symmetry setting



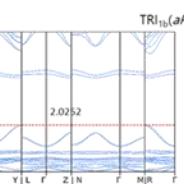
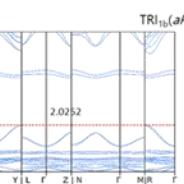
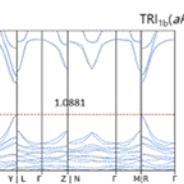
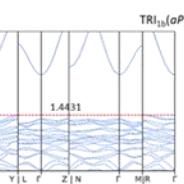
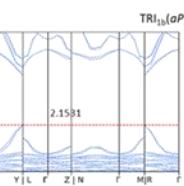
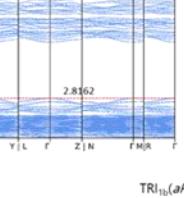
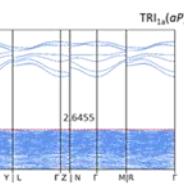
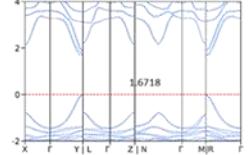
P1 setting



Original symmetry setting



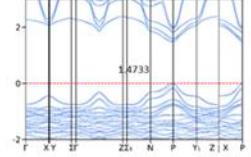
P1 setting



## NSAG-III 4<sup>th</sup> Generation

Original symmetry setting

**49  $(C_2OH_5)_3Ge_2I_7$**



*P1* setting

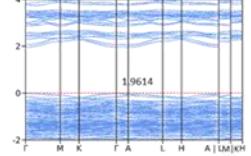
BCT<sub>2</sub>(tf)

Original symmetry setting

*P1* setting

TRI<sub>13</sub>(oP)

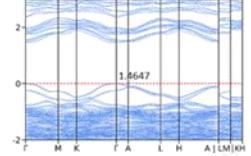
**50  $(CH_3C(NH_2)_2)GeI_3$**



HEX(hP)

TRI<sub>13</sub>(oP)

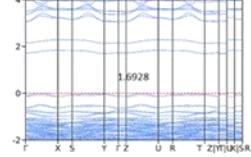
**51  $((CH_3)_2NH_2)SnI_3$**



HEX(hP)

TRI<sub>13</sub>(oP)

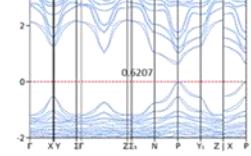
**52  $(CH_3CH_2NH_3)InBr_3$**



ORC(oP)

TRI<sub>13</sub>(oP)

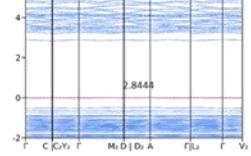
**53  $(C_2OH_5)_3Sn_2I_7$**



BCT<sub>2</sub>(tf)

TRI<sub>13</sub>(oP)

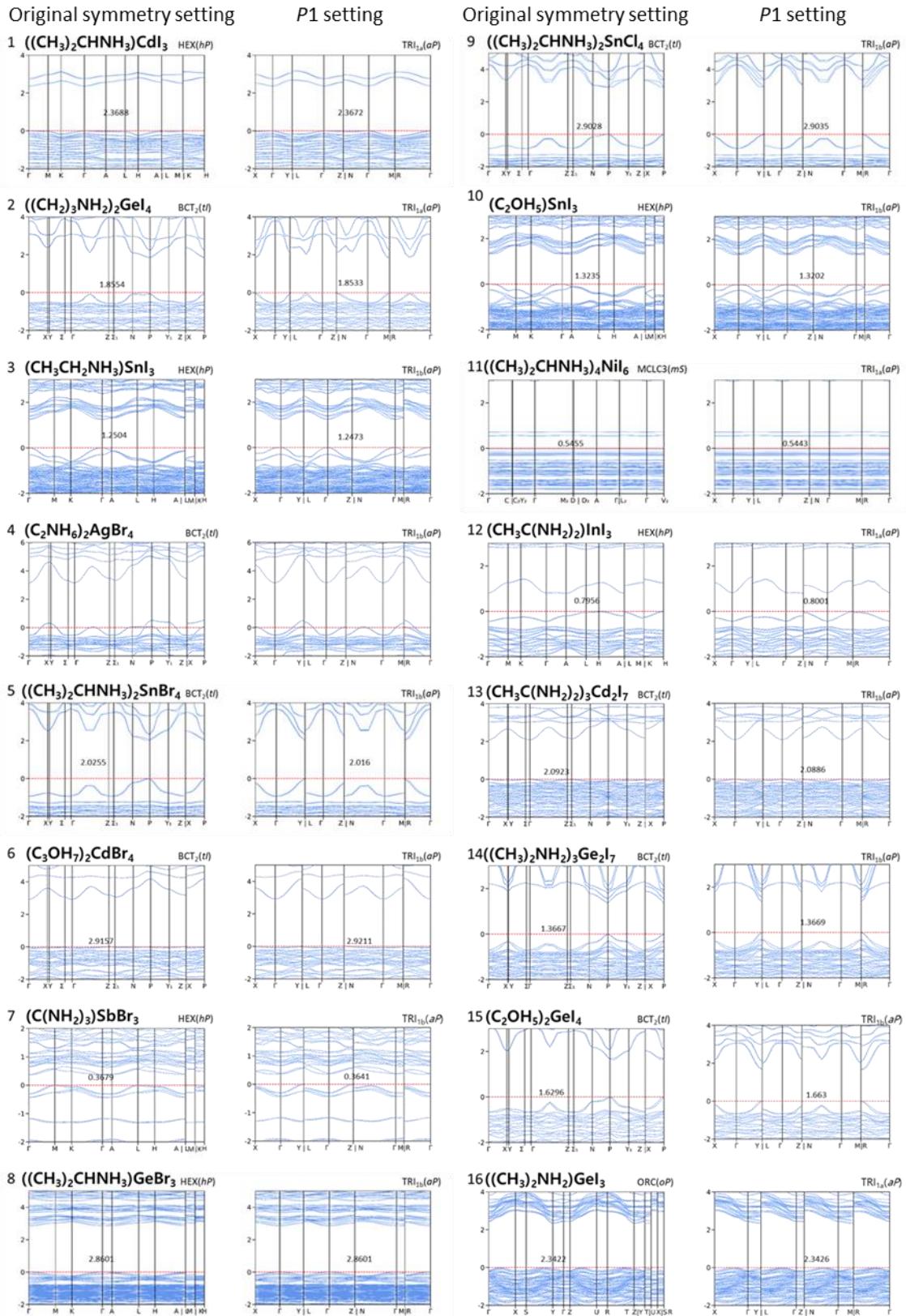
**54  $(C_3OH_7)_4SnBr_6$**



MCLC3(mS)

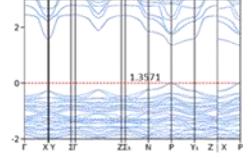
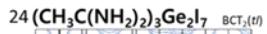
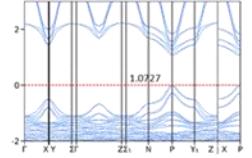
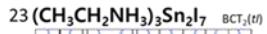
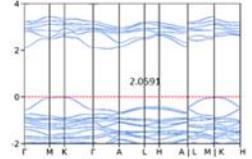
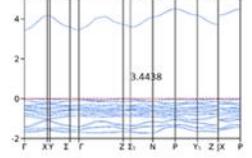
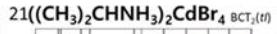
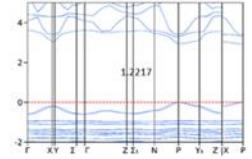
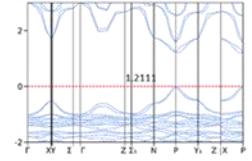
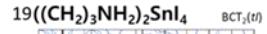
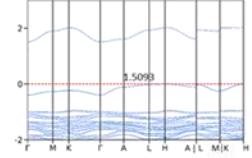
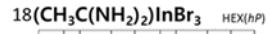
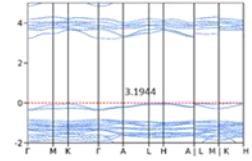
TRI<sub>13</sub>(oP)

## NSAG-III 5<sup>th</sup> Generation

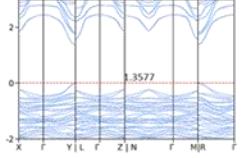
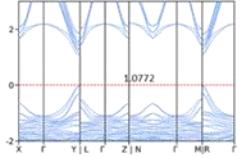
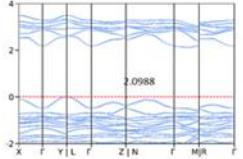
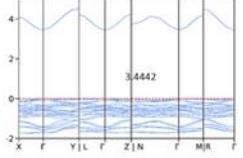
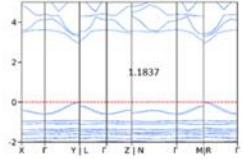
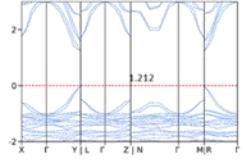
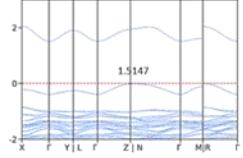
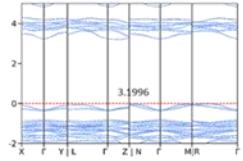
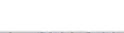


## NSAG-III 5<sup>th</sup> Generation

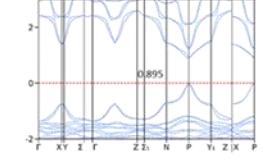
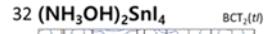
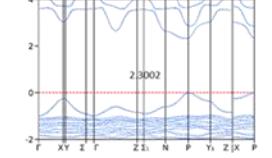
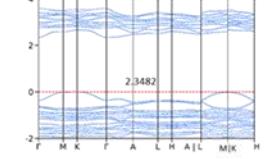
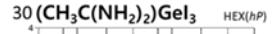
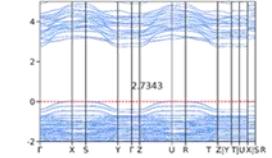
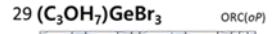
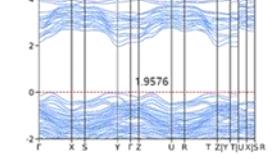
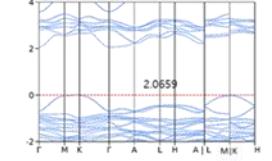
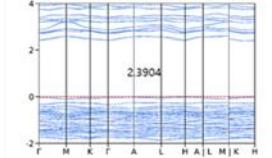
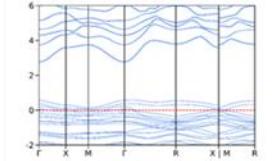
Original symmetry setting



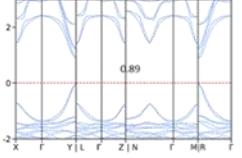
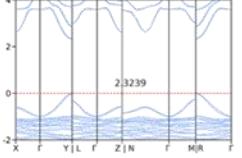
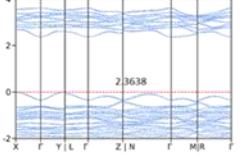
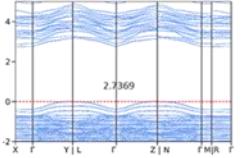
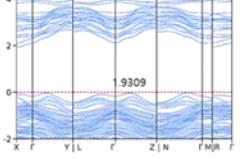
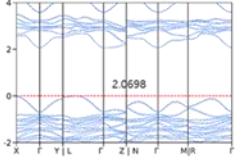
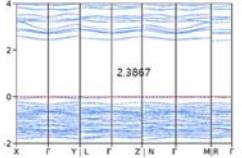
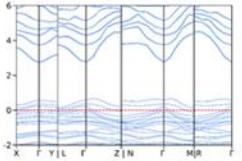
*P1* setting



Original symmetry setting

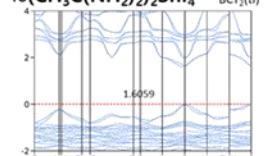
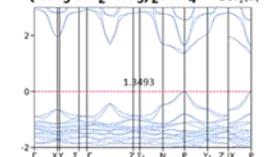
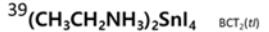
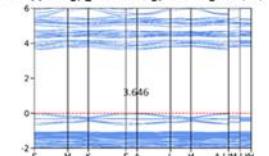
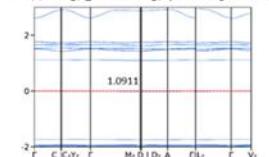
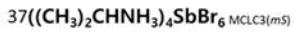
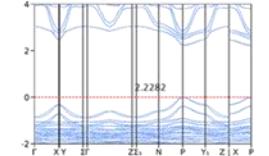
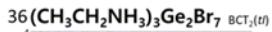
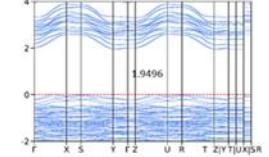
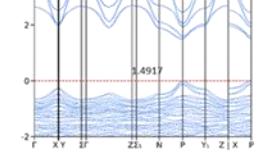
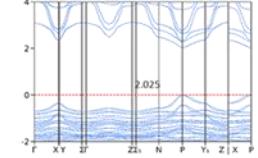
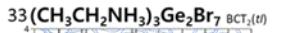


*P1* setting

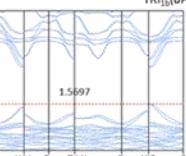
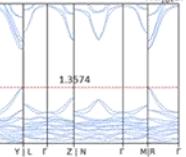
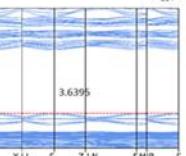
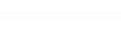
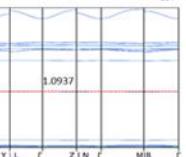
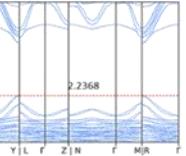
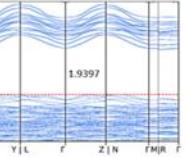
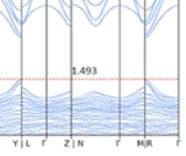
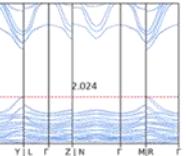


## NSAG-III 5<sup>th</sup> Generation

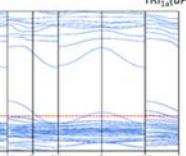
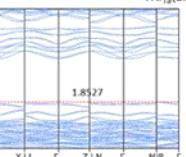
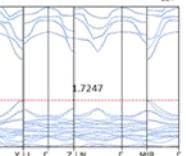
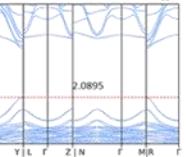
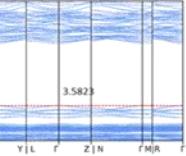
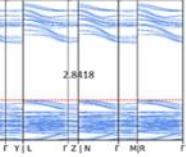
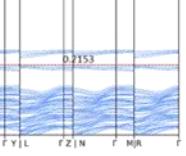
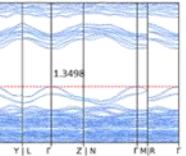
Original symmetry setting



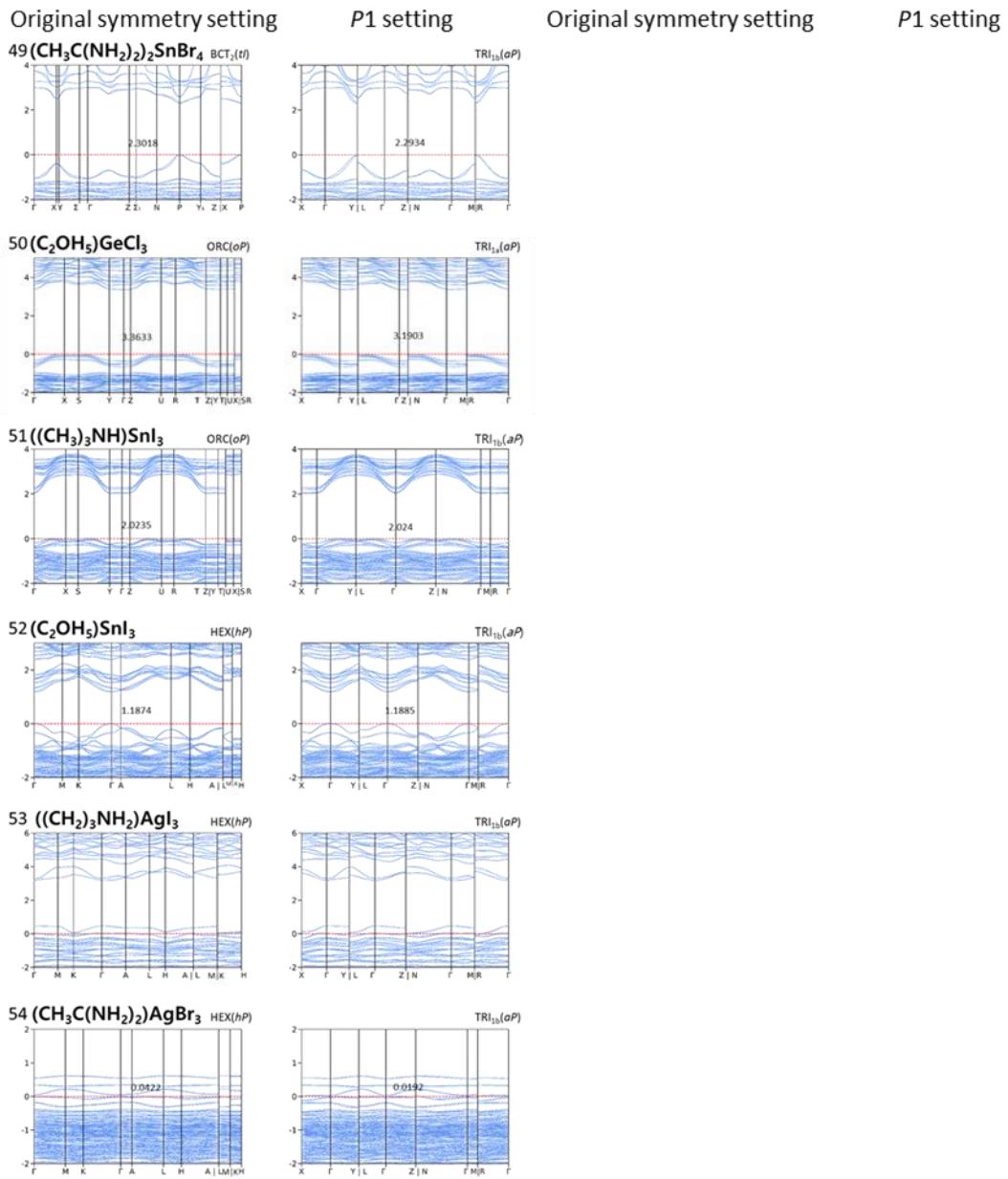
P1 setting



P1 setting



## NSAG-III 5<sup>th</sup> Generation



**Figure S4.** The band structures (E-k plots) for both the original and *P1* symmetry settings for every generation in the NSGA-II and –III process. The band gap values are presented if available.

**Table S1.** The effect of the molecular orientation on the DFT-calculated total energy, band gap, and the effective mass for 27 random initial ‘A’-site molecular orientations for  $(\text{NH}_3\text{OH})\text{PbCl}_3$  and  $(\text{CH}_3\text{NH}_3)\text{Cl}$ . Two different symmetry settings were adopted for band structure calculations, Bravais lattice setting in the left side and primitive  $P1$  setting in the right side. The molecules are numbered identically to that shown in Figure S1.

#	Total energy	$(\text{NH}_3\text{OH})\text{PbCl}_3$						$(\text{CH}_3\text{NH}_3)\text{Cl}$					
		Bravais lattic setting			$P1$ setting			Total energy	Bravais lattic setting			$P1$ setting	
		$E_g^{\text{GGA}}$	$m_e^*$	$m_h^*$	$E_g^{\text{GGA}}$	$m_e^*$	$m_h^*$		$E_g^{\text{GGA}}$	$m_e^*$	$m_h^*$	$E_g^{\text{GGA}}$	$m_e^*$
1	-42.8476	2.55	0.99	0.82	2.55	0.13	0.82	-43.4866	5.17	1.45	0.71	5.17	1.45
2	-42.8459	2.56	0.97	2.53	2.48	0.94	0.74	-43.6128	5.20	3.89	0.82	5.22	0.14
3	-42.8458	2.52	1.00	0.76	2.52	0.13	0.76	-43.4940	5.15	5.50	0.75	5.16	7.62
4	-42.8481	2.46	1.00	0.68	2.52	0.13	0.75	-43.4881	5.18	1.49	0.75	5.18	1.49
5	-42.8476	2.58	0.99	1.03	2.51	0.96	0.75	-43.4823	5.17	3.51	0.72	5.17	3.51
6	-42.8469	2.48	0.12	1.46	2.54	0.12	0.83	-43.4871	5.18	1.47	0.76	5.18	1.47
7	-42.8469	2.52	0.13	0.75	2.52	0.13	0.75	-43.4992	5.15	3.97	0.71	5.15	6.82
8	-42.8477	2.46	0.12	1.44	2.53	1.71	0.97	-43.4536	5.20	2.61	0.78	5.20	2.61
9	-42.8469	2.53	0.13	0.96	2.53	0.13	0.96	-43.4533	5.19	0.27	0.74	5.20	3.19
10	-42.8468	2.58	0.99	1.04	2.51	0.95	0.75	-43.4902	5.20	69.43	0.71	5.17	7.37
11	-42.8472	2.45	0.99	0.68	2.51	0.13	0.75	-43.4535	5.20	3.47	0.74	5.20	3.47
12	-42.8469	2.56	1.01	0.83	2.56	0.13	0.83	-43.4536	5.20	3.42	0.76	5.20	3.42
13	-42.8462	2.47	1.01	0.69	2.58	0.13	1.04	-43.4849	5.18	1.89	0.80	5.18	1.89
14	-42.8468	2.52	0.13	0.75	2.52	0.13	0.75	-43.4844	5.16	4.14	0.76	5.18	1.80
15	-42.8468	2.57	0.13	1.03	2.57	0.13	1.03	-43.4536	5.20	4.30	0.75	5.20	4.12
16	-42.8470	2.51	0.13	0.75	2.51	0.13	0.75	-43.4535	5.20	4.26	0.79	5.20	3.55
17	-42.8479	2.51	0.12	1.56	2.59	0.12	1.06	-43.4973	5.17	7.12	0.76	5.17	7.12
18	-42.8472	2.50	0.12	1.53	2.52	0.12	0.76	-43.4960	5.15	4.96	0.74	5.16	8.93
19	-42.8470	2.66	0.13	3.09	2.54	0.93	0.91	-43.4532	5.20	4.21	0.78	5.20	4.33
20	-42.8471	2.48	0.12	1.46	2.55	0.12	0.82	-43.4859	5.17	1.64	0.80	5.17	1.64
21	-42.8468	2.53	0.13	0.96	2.53	0.13	0.96	-43.4533	5.20	4.54	0.73	5.20	3.58
22	-42.8482	2.55	0.13	0.83	2.55	0.13	0.83	-43.4832	5.16	4.47	0.76	5.17	2.93
23	-42.8468	2.49	0.12	1.45	2.57	2.01	1.01	-43.4851	5.16	5.42	0.78	5.17	1.78
24	-42.8473	2.48	0.13	1.45	2.54	0.13	0.83	-43.5422	5.16	7.93	0.75	5.16	7.20
25	-42.8470	2.66	0.13	3.33	2.54	0.94	0.90	-43.4953	5.15	3.97	0.79	5.16	7.90
26	-42.8469	2.56	0.13	1.01	2.56	0.13	1.01	-43.4532	5.20	6.00	0.76	5.20	3.35
27	-42.8467	2.46	0.12	0.68	2.51	0.12	0.75	-43.4935	5.19	5.64	0.73	5.16	7.50

**Table S2.** The DFT-calculated total energy for all the hypothetical MX compounds used for the reaction (formation) energy calculation.

#	MX compounds	Total energy (eV)		
		-Cl	-Br	-I
1	NH <sub>4</sub>	-27.51	-	-26.56
2	CH <sub>3</sub> NH <sub>3</sub>	-43.92	-43.38	-42.78
3	NH <sub>3</sub> NH <sub>2</sub>	-38.53	-37.90	-37.43
4	NH <sub>3</sub> OH	-32.45	-32.03	-31.37
5	C <sub>2</sub> NH <sub>6</sub>	-51.59	-51.06	-50.47
6	CH(NH <sub>2</sub> ) <sub>2</sub>	-48.71	-48.18	-47.60
7	C <sub>2</sub> OH <sub>5</sub>	-45.05	-44.43	-43.82
8	(CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub>	-60.23	-59.73	-59.18
9	CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub>	-60.65	-60.08	-59.48
10	(CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub>	-68.47	-67.94	-67.35
11	CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub>	-65.53	-64.92	-64.23
12	C <sub>3</sub> OH <sub>7</sub>	-61.92	-61.34	-60.71
13	(CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub>	-71.30	-70.78	-70.46
14	(CH <sub>3</sub> ) <sub>3</sub> NH	-76.36	-75.87	-75.33
15	C(NH <sub>2</sub> ) <sub>3</sub>	-61.52	-60.41	-60.24
16	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>3</sub>	-77.21	-76.60	-76.05
17	C <sub>4</sub> NH <sub>10</sub>	-69.25	-68.65	-67.99
18	C <sub>3</sub> N <sub>2</sub> H <sub>5</sub>	-	-65.64	-
19	NC <sub>4</sub> H <sub>8</sub>	-76.52	-75.89	-
20	C(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>	-84.16	-83.65	-
21	C <sub>4</sub> NH <sub>10</sub>	-85.80	-85.30	-
22	C <sub>4</sub> OH <sub>9</sub>	-79.32	-78.65	-
23	(CH <sub>3</sub> ) <sub>4</sub> N	-92.23	-91.89	-
24	(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>2</sub> ) <sub>2</sub> NH <sub>2</sub>	-	-	-
25	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> NH <sub>3</sub>	-93.93	-	-
26	C <sub>3</sub> H <sub>4</sub> NS	-57.44	-	-
27	C <sub>5</sub> NH <sub>12</sub>	-102.70	-	-
28	C <sub>5</sub> OH <sub>11</sub>	-95.98	-	-
29	C <sub>4</sub> H <sub>11</sub> N <sub>2</sub>	-98.80	-	-
30	NH(CH <sub>2</sub> ) <sub>3</sub> S	-	-	-
31	C <sub>7</sub> H <sub>7</sub>	-91.95	-	-
32	C(CH) <sub>5</sub> NH <sub>3</sub>	-	-	-
33	C <sub>6</sub> NH <sub>14</sub>	-119.06	-	-
34	C <sub>6</sub> OH <sub>13</sub>	-	-	-

**Table S3.** The DFT-calculated total energy for all the real and hypothetical BX<sub>2</sub> compounds used for the reaction (formation) energy calculation. Real and hypothetical BX<sub>2</sub> structures are discerned using colors (blue font for hypothetical).

#	Atoms	BX <sub>2</sub> compounds total energy (eV)			#	Atoms	BX <sub>2</sub> compounds total energy (eV)		
		-Cl	-Br	-I			-Cl	-Br	-I
1	Be	-12.05	-10.54	-9.02	22	Rh	-	-11.93	-11.35
2	Mg	-11.21	-9.85	-8.35	23	Pd	-10.93	-10.16	-9.79
3	Si	-12.39	-11.07	-9.89	24	Ag	-7.89	-7.41	-6.96
4	P	-	-10.06	-9.17	25	Cd	-8.17	-7.25	-9.86
5	Ca	-13.25	-11.85	-	26	In	-9.78	-8.79	-7.79
6	Sc	-15.99	-14.69	-13.29	27	Sn	-10.98	-10.00	-9.01
7	Ti	-16.29	-	-13.43	28	Sb	-10.21	-9.12	-9.12
8	V	-15.90	-14.46	-13.07	29	Ba	-13.66	-12.40	-
9	Mn	-14.29	-13.09	-12.12	30	Sm	-14.42	-13.42	-12.17
10	Fe	-13.67	-12.58	-11.72	31	Eu	-22.40	-	-
11	Co	-12.22	-11.28	-10.53	32	Tm	-14.00	-12.61	-11.58
12	Ni	-10.76	-9.95	-9.26	33	Yb	-13.25	-11.73	-10.19
13	Zn	-8.65	-7.62	-6.57	34	Hf	-18.64	-18.04	-
14	Ge	-10.94	-10.01	-9.19	35	Ta	-19.92	-18.70	-
15	As	-10.51	-9.07	-8.65	36	W	-20.11	-19.13	-18.33
16	Sr	-13.26	-11.89	-10.41	37	Re	-17.84	-	-
17	Cu	-9.30	-8.48	-7.83	38	Pt	-11.55	-10.81	-
18	Y	-	-15.15	-13.85	39	Au	-8.62	-7.89	-
19	Zr	-17.80	-16.18	-15.02	40	Hg	-6.43	-5.74	-5.37
20	Nb	-17.88	-16.62	-15.34	41	Tl	-8.89	-8.04	-
21	Mo	-17.97	-16.89	-15.83	42	Bi	-	-	-

**Table S4.** The decision variable and objective function values for all the entries belonging to the 1<sup>st</sup> ~ 5<sup>th</sup> generations for NSGA-II.

#	Chemical Formula	Decision Variables				Objective function Values	
		A	B	X	S	Obj_E <sub>g</sub>	Obj_E <sub>f</sub>
1	(C <sub>5</sub> NH <sub>12</sub> )HfCl <sub>3</sub>	27	34	1	2	0.54	0.004
2	(CH(NH <sub>2</sub> ) <sub>2</sub> )SmCl <sub>3</sub>	6	30	1	8	Metal	-0.015
3	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )AgBr <sub>3</sub>	10	24	2	4	1.54	0.015
4	(C <sub>7</sub> H <sub>7</sub> ) <sub>2</sub> ReCl <sub>4</sub>	31	37	1	3	0.24	0.080
5	(C <sub>2</sub> NH <sub>6</sub> ) <sub>4</sub> GeI <sub>6</sub>	5	14	3	10	3.18	0.005
6	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> ) <sub>3</sub> Ta <sub>2</sub> Cl <sub>7</sub>	10	35	1	5	0.15	0.139
7	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )Mo <sub>4</sub> I <sub>9</sub>	10	21	3	9	0.10	0.174
8	(CH <sub>3</sub> NH <sub>3</sub> ) <sub>2</sub> BeI <sub>4</sub>	2	1	3	3	3.80	0.015
9	(C <sub>3</sub> OH <sub>7</sub> )AgBr <sub>3</sub>	12	24	2	2	Metal	0.047
10	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )MnI <sub>3</sub>	9	9	3	2	Metal	0.054
11	(C <sub>6</sub> NH <sub>14</sub> )Pt <sub>4</sub> Cl <sub>9</sub>	33	38	1	9	0.80	0.032
12	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> ScI <sub>4</sub>	11	6	3	3	failure	
13	(NH <sub>3</sub> OH) <sub>4</sub> YbCl <sub>6</sub>	4	33	1	7	5.21	-0.010
14	(CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>3</sub> )SmI <sub>3</sub>	16	30	3	4	Metal	0.022
15	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )AgCl <sub>3</sub>	9	24	1	1	Metal	0.034
16	(C <sub>3</sub> H <sub>4</sub> NS) <sub>2</sub> VCl <sub>4</sub>	26	8	1	3	failure	
17	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>4</sub> BeCl <sub>6</sub>	13	1	1	7	failure	
18	(CH(NH <sub>2</sub> ) <sub>2</sub> ) <sub>4</sub> HgI <sub>6</sub>	6	40	3	10	1.94	0.000
19	(C <sub>2</sub> OH <sub>5</sub> ) <sub>3</sub> CaBr <sub>6</sub>	7	5	2	7	3.91	-0.002
20	(C <sub>2</sub> OH <sub>5</sub> )GeCl <sub>3</sub>	7	14	1	1	2.55	-0.018
21	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )BeI <sub>3</sub>	8	1	3	8	3.69	0.007
22	(NH <sub>3</sub> OH)SrI <sub>3</sub>	4	16	3	6	3.73	0.043
23	(C <sub>2</sub> NH <sub>6</sub> )MgI <sub>3</sub>	5	2	3	1	2.22	0.014
24	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> ZrI <sub>6</sub>	11	19	3	7	Metal	0.019
25	(NH <sub>4</sub> ) <sub>4</sub> TlI <sub>6</sub>	1	7	3	10	Metal	0.024
26	(CH(NH <sub>2</sub> ) <sub>2</sub> )SrBr <sub>3</sub>	6	16	2	4	4.33	-0.119
27	(C <sub>3</sub> N <sub>2</sub> H <sub>5</sub> )WCl <sub>3</sub>	18	36	1	4	failure	
28	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )BeI <sub>3</sub>	11	1	3	2	3.68	-0.027
29	(C(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>3</sub> Re <sub>2</sub> Cl <sub>7</sub>	20	37	1	5	failure	
30	(C(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> TaCl <sub>4</sub>	20	35	1	3	0.10	-0.011
31	(C <sub>4</sub> NH <sub>10</sub> )TmCl <sub>3</sub>	21	32	1	8	Metal	-0.082
32	(NH <sub>4</sub> ) <sub>3</sub> Cu <sub>2</sub> I <sub>7</sub>	1	17	3	5	Metal	0.029
33	(C <sub>5</sub> NH <sub>12</sub> ) <sub>3</sub> Pt <sub>2</sub> Cl <sub>7</sub>	27	38	1	5	failure	
34	(C <sub>3</sub> N <sub>2</sub> H <sub>5</sub> )Tm <sub>4</sub> Br <sub>9</sub>	18	32	2	9	Metal	-0.032
35	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )SiBr <sub>3</sub>	8	3	2	4	2.92	0.056
36	(CH <sub>3</sub> NH <sub>3</sub> )PdCl <sub>3</sub>	2	23	1	8	1.15	0.010
37	(C <sub>4</sub> NH <sub>10</sub> )BaBr <sub>3</sub>	21	29	2	1	4.45	0.004
38	(C <sub>7</sub> H <sub>7</sub> ) <sub>2</sub> Ba <sub>2</sub> Br <sub>7</sub>	31	29	2	5	failure	
39	(NH <sub>3</sub> OH)RhBr <sub>3</sub>	4	22	2	1	Metal	0.083
40	(C <sub>3</sub> N <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> MoBr <sub>6</sub>	18	21	2	7	failure	
41	(NH <sub>3</sub> NH <sub>2</sub> ) <sub>5</sub> SmBr <sub>6</sub>	3	30	2	7	0.02	0.023
42	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )TiBr <sub>3</sub>	10	41	2	2	0.99	0.003
43	(C <sub>2</sub> OH <sub>5</sub> ) <sub>2</sub> PtBr <sub>4</sub>	7	38	2	3	Metal	0.035
44	(C <sub>3</sub> N <sub>2</sub> H <sub>5</sub> )PtBr <sub>3</sub>	18	38	2	6	0.52	0.034
45	(C <sub>4</sub> OH <sub>5</sub> )RhBr <sub>3</sub>	22	22	2	2	Metal	0.022
46	((CH <sub>3</sub> ) <sub>4</sub> N) <sub>2</sub> AuBr <sub>4</sub>	23	39	2	3	Metal	0.003
47	((CH <sub>3</sub> ) <sub>3</sub> NH)GeI <sub>3</sub>	14	14	3	2	2.52	-0.007
48	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )MgI <sub>3</sub>	8	2	3	1	1.28	0.037
49	(CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>3</sub> )SrI <sub>3</sub>	16	16	3	1	2.82	0.072
50	(C <sub>4</sub> OH <sub>5</sub> )FeBr <sub>3</sub>	22	10	2	8	0.28	0.037

#	Chemical Formula	Decision Variables				Objective function Values	
		A	B	X	S	Obj_Eg	Obj_Ef
1	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )PI <sub>3</sub>	9	4	3	2	0.48	0.040
2	(C(NH <sub>2</sub> ) <sub>3</sub> )EuBr <sub>3</sub>	15	31	2	2	Metal	-0.025
3	(C <sub>2</sub> OH <sub>5</sub> ) <sub>2</sub> Gel <sub>4</sub>	7	14	3	3	0.13	0.004
4	(NC <sub>4</sub> H <sub>8</sub> )PtBr <sub>3</sub>	19	38	2	6		Failure
5	(NH <sub>3</sub> OH)MgI <sub>3</sub>	4	2	3	1	0.32	0.058
6	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )FeBr <sub>3</sub>	9	10	2	1	Metal	0.082
7	(NC <sub>4</sub> H <sub>8</sub> )Fe <sub>4</sub> Cl <sub>9</sub>	19	10	1	9	1.42	0.162
8	(C <sub>2</sub> OH <sub>5</sub> )PBr <sub>3</sub>	7	4	2	6	0.91	0.071
9	(C <sub>2</sub> NH <sub>6</sub> )YbI <sub>3</sub>	5	33	3	8	2.22	0.000
10	(C <sub>5</sub> NH <sub>12</sub> ) <sub>3</sub> Hf <sub>2</sub> Cl <sub>7</sub>	27	34	1	5	1.24	0.078
11	(C <sub>2</sub> N <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NbBr <sub>6</sub>	18	20	2	7	Metal	0.073
12	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )AgI <sub>3</sub>	10	24	3	1	Metal	0.021
13	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>4</sub> PdBr <sub>6</sub>	8	23	2	7	0.15	0.024
14	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>4</sub> NbBr <sub>6</sub>	13	20	2	7	Metal	0.055
15	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )NiBr <sub>3</sub>	13	12	2	4		Failure
16	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )HgBr <sub>3</sub>	8	40	2	4	0.55	0.005
17	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )NbCl <sub>3</sub>	9	20	1	1	Metal	0.170
18	(C(CH <sub>3</sub> ) <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub> )TaCl <sub>3</sub>	20	35	1	4	Metal	0.018
19	(C <sub>2</sub> NH <sub>6</sub> )ZrBr <sub>3</sub>	5	19	2	8	1.35	0.061
20	(CH <sub>3</sub> NH <sub>3</sub> )CuI <sub>3</sub>	2	17	3	6	Metal	0.023
21	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )YbBr <sub>3</sub>	8	33	2	2	3.26	0.001
22	(C(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> )TaCl <sub>3</sub>	20	35	1	2	Metal	0.023
23	(CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> NH <sub>3</sub> )SbCl <sub>3</sub>	25	28	1	8	Metal	0.005
24	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>3</sub> Mg <sub>2</sub> Cl <sub>7</sub>	13	2	1	5	3.57	0.011
25	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> ) <sub>2</sub> ZrCl <sub>6</sub>	10	19	1	7	Metal	0.055
26	(NH <sub>3</sub> NH <sub>2</sub> )Ge <sub>4</sub> I <sub>9</sub>	3	14	3	9	0.81	0.012
27	(NH <sub>3</sub> OH)FeBr <sub>3</sub>	4	10	2	6	1.50	0.091
28	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )AgI <sub>3</sub>	10	24	3	2	Metal	0.008
29	(C <sub>4</sub> NH <sub>10</sub> ) <sub>2</sub> TaCl <sub>4</sub>	17	35	1	3	1.35	0.116
30	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>3</sub> P <sub>2</sub> Br <sub>7</sub>	8	4	2	5	Metal	0.064
31	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )CdI <sub>3</sub>	11	25	3	2	0.64	0.233
32	(C <sub>4</sub> NH <sub>10</sub> )ZrBr <sub>3</sub>	17	19	2	4	Metal	0.022
33	(C <sub>2</sub> OH <sub>5</sub> ) <sub>3</sub> V <sub>2</sub> Br <sub>7</sub>	7	8	2	5	Metal	0.079
34	(C(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>3</sub> Ni <sub>2</sub> Br <sub>7</sub>	20	12	2	5	1.10	-0.024
35	(C(NH <sub>2</sub> ) <sub>3</sub> )Mol <sub>3</sub>	15	21	3	2	Metal	0.137
36	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )MnI <sub>3</sub>	9	9	3	1	Metal	0.053
37	(NH <sub>3</sub> NH <sub>2</sub> )MgI <sub>3</sub>	3	2	3	6	0.55	0.047
38	(C <sub>4</sub> NH <sub>10</sub> )PtCl <sub>3</sub>	21	38	1	8	0.32	-0.090
39	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )BaBr <sub>3</sub>	11	29	2	6	2.62	0.001
40	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )EuCl <sub>3</sub>	8	31	1	6		Failure
41	(CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>3</sub> )Re <sub>2</sub> Cl <sub>7</sub>	16	37	1	5	0.92	0.097
42	(C <sub>3</sub> OH <sub>7</sub> ) <sub>3</sub> Sn <sub>2</sub> Cl <sub>7</sub>	12	27	1	5	0.93	-0.001
43	(NH <sub>3</sub> NH <sub>2</sub> ) <sub>3</sub> V <sub>2</sub> I <sub>7</sub>	3	8	3	5	Metal	0.046
44	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )CuI <sub>3</sub>	9	17	3	8	Metal	0.026
45	(C <sub>3</sub> NS) <sub>4</sub> BaCl <sub>6</sub>	26	29	1	7		Failure
46	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )NiI <sub>3</sub>	9	12	3	8	1.42	0.015
47	(C <sub>2</sub> NH <sub>6</sub> ) <sub>4</sub> NbI <sub>6</sub>	5	20	3	7	Metal	0.055
48	(NH <sub>3</sub> NH <sub>2</sub> ) <sub>4</sub> SiI <sub>6</sub>	3	3	3	7	0.92	0.018
49	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )ZrI <sub>3</sub>	10	19	3	6	Metal	0.085
50	(C <sub>3</sub> OH <sub>7</sub> )Tm <sub>4</sub> Cl <sub>9</sub>	12	32	1	9	Metal	-0.027
51	(C <sub>2</sub> NH <sub>6</sub> )SrBr <sub>3</sub>	5	16	2	1	3.18	0.009
52	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )Ba <sub>4</sub> Br <sub>9</sub>	13	29	2	9	2.62	0.049
53	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )ScCl <sub>3</sub>	11	6	1	1	Metal	0.043
54	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )Sm <sub>4</sub> Br <sub>9</sub>	8	30	2	9	1.48	0.000

#	Chemical Formula	Decision Variables				Objective function Values	
		A	B	X	S	Obj_Eg	Obj_Ef
1	(C(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> )Yb <sub>4</sub> Cl <sub>9</sub>	20	33	1	9	0.28	0.02
2	(C <sub>2</sub> NH <sub>6</sub> )InI <sub>3</sub>	5	26	3	8	Metal	0.01
3	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>3</sub> Ni <sub>2</sub> I <sub>7</sub>	13	12	3	5		Failure
4	(C(NH <sub>2</sub> ) <sub>3</sub> )SnBr <sub>3</sub>	14	27	2	8	0.96	-0.033
5	(CH(NH <sub>2</sub> ) <sub>2</sub> )ZnI <sub>3</sub>	6	13	3	8	1.08	0.014
6	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )YI <sub>3</sub>	11	18	3	8	Metal	0.001
7	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>4</sub> YbBr <sub>6</sub>	8	33	2	7	2.98	0.012
8	(C <sub>2</sub> OH <sub>5</sub> ) <sub>4</sub> CoI <sub>6</sub>	7	11	3	7	1.41	0.119
9	((CH <sub>3</sub> ) <sub>3</sub> NH)Y <sub>4</sub> I <sub>9</sub>	14	18	3	9	Metal	0.026
10	(NH <sub>3</sub> NH <sub>2</sub> ) <sub>4</sub> GeCl <sub>6</sub>	3	14	1	7	2.53	-0.010
11	(C <sub>2</sub> OH <sub>5</sub> ) <sub>3</sub> Yb <sub>2</sub> Cl <sub>7</sub>	7	33	1	5	3.02	0.014
12	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>3</sub> Sb <sub>2</sub> Cl <sub>7</sub>	8	28	1	5	Metal	0.037
13	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>4</sub> VBr <sub>6</sub>	8	8	2	7	1.24	0.084
14	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>4</sub> CaBr <sub>6</sub>	11	5	2	7	2.25	-0.014
15	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )InI <sub>3</sub>	8	26	3	4	0.01	0.023
16	(CH(NH <sub>2</sub> ) <sub>2</sub> ) <sub>4</sub> BaCl <sub>6</sub>	6	29	1	7	2.69	0.022
17	(C <sub>3</sub> NH <sub>6</sub> ) <sub>3</sub> Sm <sub>2</sub> Cl <sub>7</sub>	5	30	1	5	Metal	0.005
18	(C(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> HfCl <sub>4</sub>	20	34	1	3	0.90	-0.028
19	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )VCl <sub>3</sub>	9	8	1	4	1.44	0.057
20	((CH <sub>3</sub> ) <sub>3</sub> NH)ZrCl <sub>3</sub>	14	19	1	1	0.67	0.119
21	((CH <sub>2</sub> ) <sub>3</sub> NH) <sub>2</sub> GeBr <sub>3</sub>	10	14	2	8	1.40	-0.008
22	((CH <sub>3</sub> ) <sub>3</sub> NH)SbCl <sub>3</sub>	14	28	1	8	Metal	-0.003
23	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )VI <sub>3</sub>	8	8	3	8	Metal	0.024
24	(C(NH <sub>2</sub> ) <sub>3</sub> ) <sub>2</sub> GeBr <sub>4</sub>	15	14	2	3	1.17	-0.048
25	(C <sub>2</sub> OH <sub>5</sub> ) <sub>3</sub> MnBr <sub>3</sub>	7	30	2	6		Failure
26	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )YBr <sub>3</sub>	8	18	2	8	Metal	0.017
3 <sup>rd</sup> Gen.	(C(NH <sub>2</sub> ) <sub>3</sub> ) <sub>4</sub> HfBr <sub>6</sub>	15	34	2	7	1.30	0.004
	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> AgBr <sub>4</sub>	8	24	2	3	Metal	0.011
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )GeI <sub>3</sub>	9	14	3	6	0.28	0.009
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>3</sub> Y <sub>2</sub> Br <sub>7</sub>	13	18	2	5		Failure
	(C <sub>4</sub> OH <sub>5</sub> ) <sub>3</sub> Ta <sub>2</sub> Cl <sub>7</sub>	22	35	1	5	1.38	0.158
	(C <sub>2</sub> NH <sub>6</sub> )YbBr <sub>3</sub>	5	33	2	4	2.93	0.008
	(C(NH <sub>2</sub> ) <sub>3</sub> ) <sub>3</sub> FeI <sub>7</sub>	15	10	3	5	1.42	0.047
	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )SrI <sub>3</sub>	8	16	3	8	2.23	0.019
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>4</sub> TmBr <sub>6</sub>	13	32	2	10	1.99	-0.021
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )TmBr <sub>3</sub>	13	32	2	8	Metal	-0.003
	(C <sub>2</sub> NH <sub>6</sub> ) <sub>4</sub> MnBr <sub>6</sub>	5	9	2	7	0.88	0.044
	(C <sub>2</sub> NH <sub>6</sub> ) <sub>4</sub> YbBr <sub>6</sub>	5	33	2	7	3.31	0.007
	((CH <sub>3</sub> ) <sub>4</sub> N)TaCl <sub>3</sub>	23	35	1	2	0.43	0.031
	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )FeBr <sub>3</sub>	8	10	2	2	0.88	0.021
	(C <sub>3</sub> OH <sub>7</sub> )AgBr <sub>3</sub>	12	24	2	1	Metal	0.032
	(C <sub>2</sub> NH <sub>6</sub> )YI <sub>3</sub>	5	18	3	8	Metal	0.009
	(C <sub>4</sub> NH <sub>10</sub> )TiBr <sub>3</sub>	17	41	2	6	0.59	-0.004
	(C <sub>2</sub> NH <sub>6</sub> ) <sub>4</sub> CaBr <sub>6</sub>	5	5	2	7	3.30	0.006
	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )HgI <sub>6</sub>	8	40	3	10	0.37	0.011
46	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> SiI <sub>4</sub>	8	3	3	3	0.41	0.036
47	(C <sub>3</sub> N <sub>2</sub> H <sub>5</sub> )BaBr <sub>3</sub>	18	29	2	1	1.91	0.035
48	(NH <sub>3</sub> NH <sub>2</sub> )SrI <sub>3</sub>	3	16	3	6	2.31	0.019
49	(C <sub>2</sub> NH <sub>6</sub> )Ag <sub>4</sub> Br <sub>9</sub>	5	24	2	9	Metal	-0.013
50	(C <sub>2</sub> H <sub>7</sub> )ReCl <sub>3</sub>	31	37	1	4		Failure
51	(C <sub>4</sub> H <sub>11</sub> N <sub>2</sub> )HfCl <sub>3</sub>	29	34	1	2	1.21	0.067
52	(NH <sub>3</sub> OH)SiI <sub>3</sub>	4	3	3	8	0.18	0.091
53	(CH(NH <sub>2</sub> ) <sub>2</sub> )Ge <sub>4</sub> I <sub>9</sub>	6	14	3	9	0.82	0.008
54	(CH(NH <sub>2</sub> ) <sub>2</sub> )CuBr <sub>3</sub>	6	17	2	6	Metal	0.005

#	Chemical Formula	Decision Variables				Objective function Values	
		A	B	X	S	Obj_Eg	Obj_Ef
1	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )ZrBr <sub>3</sub>	8	19	2	6	Metal	0.084
2	(C <sub>3</sub> O <sub>H</sub> )SrI <sub>3</sub>	12	16	3	2	2.25	0.004
3	(NH <sub>3</sub> OH)SrBr <sub>3</sub>	4	16	2	4	2.73	0.030
4	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )CoBr <sub>3</sub>	13	11	2	6	Failure	
5	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>4</sub> MnI <sub>6</sub>	13	9	3	7	0.99	0.046
6	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )RhI <sub>3</sub>	11	22	3	6	Metal	0.024
7	(NH <sub>3</sub> NH <sub>2</sub> )MgI <sub>3</sub>	3	2	3	2	1.48	0.023
8	(C <sub>2</sub> O <sub>H</sub> ) <sub>5</sub> YbBr <sub>3</sub>	7	33	2	2	2.73	0.013
9	(C <sub>4</sub> NH <sub>10</sub> )BaBr <sub>3</sub>	21	29	2	2	2.66	0.028
10	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> SiCl <sub>4</sub>	9	3	1	3	1.64	0.029
11	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )CdBr <sub>3</sub>	9	25	2	4	0.86	0.012
12	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )GeI <sub>3</sub>	8	14	3	6	0.66	0.012
13	(C <sub>3</sub> O <sub>H</sub> )GeI <sub>3</sub>	12	14	3	4	0.20	0.019
14	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )SiBr <sub>3</sub>	8	3	2	1	1.10	0.036
15	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )SiBr <sub>3</sub>	9	3	2	2	0.97	0.036
16	(C <sub>2</sub> O <sub>H</sub> ) <sub>5</sub> MoI <sub>3</sub>	7	21	3	4	Metal	0.163
17	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )Hf <sub>4</sub> Br <sub>9</sub>	8	34	2	9	1.03	0.091
18	(NH <sub>3</sub> OH)GeCl <sub>3</sub>	4	14	1	6	0.84	-0.010
19	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )SiI <sub>3</sub>	8	3	3	4	0.88	0.066
20	((CH <sub>3</sub> ) <sub>3</sub> NH <sub>2</sub> ) <sub>4</sub> FeI <sub>6</sub>	10	10	3	7	1.05	0.038
21	(NH <sub>3</sub> NH <sub>2</sub> ) <sub>4</sub> ScI <sub>6</sub>	3	6	3	7	Metal	0.031
22	(CH <sub>3</sub> NH <sub>2</sub> )BeI <sub>3</sub>	2	1	3	4	1.91	0.024
23	(C <sub>3</sub> O <sub>H</sub> ) <sub>4</sub> NiBr <sub>6</sub>	12	12	2	7	1.45	0.035
24	(NC <sub>4</sub> H <sub>8</sub> )YbCl <sub>3</sub>	19	33	1	6	1.76	0.013
25	(NH <sub>3</sub> NH <sub>2</sub> )SiI <sub>3</sub>	3	3	3	6	0.68	0.163
26	(C(NH <sub>2</sub> ) <sub>3</sub> )WBr <sub>3</sub>	15	36	2	2	0.68	0.065
4 <sup>th</sup> Gen.	27 ((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )CdBr <sub>3</sub>	13	25	2	2	1.86	-0.004
	28 (NH <sub>3</sub> OH) <sub>2</sub> NiBr <sub>4</sub>	4	12	2	3	Metal	-0.001
	29 (CH(NH <sub>2</sub> ) <sub>2</sub> )ZnBr <sub>3</sub>	6	13	2	4	2.18	0.007
	30 (NH <sub>3</sub> NH <sub>2</sub> ) <sub>4</sub> NiI <sub>6</sub>	3	12	3	7	0.97	0.009
	31 ((CH <sub>3</sub> ) <sub>3</sub> NH)TaBr <sub>3</sub>	14	35	2	2	Metal	0.087
	32 (CH(NH <sub>2</sub> ) <sub>2</sub> ) <sub>3</sub> W <sub>2</sub> Br <sub>7</sub>	6	36	2	5	Metal	0.204
	33 ((CH <sub>3</sub> ) <sub>3</sub> NH)SnI <sub>3</sub>	14	27	3	4	0.47	0.003
	34 (CH(NH <sub>2</sub> ) <sub>2</sub> )AsBr <sub>3</sub>	6	15	2	6	Failure	
	35 ((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )GeBr <sub>3</sub>	13	14	2	6	1.20	-0.014
	36 ((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )SnCl <sub>3</sub>	13	27	1	2	2.21	-0.014
	37 ((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )GeI <sub>4</sub>	10	14	3	3	0.22	0.010
	38 ((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )ZnBr <sub>3</sub>	13	13	2	1	2.07	0.005
	39 (NH <sub>3</sub> NH <sub>2</sub> )BeI <sub>3</sub>	3	1	3	2	2.22	0.019
	40 ((CH <sub>3</sub> ) <sub>3</sub> NH)SiI <sub>3</sub>	14	3	3	4	0.92	0.044
	41 (CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )CdCl <sub>3</sub>	9	25	1	1	1.78	0.008
	42 ((CH <sub>3</sub> ) <sub>3</sub> NH) <sub>4</sub> SmBr <sub>6</sub>	14	30	2	10	1.59	-0.011
	43 ((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )SnI <sub>3</sub>	10	27	3	8	0.55	-0.004
	44 (CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>3</sub> Y <sub>2</sub> Br <sub>7</sub>	9	18	2	5	Metal	0.033
	45 (C <sub>2</sub> O <sub>H</sub> ) <sub>2</sub> GeBr <sub>4</sub>	7	14	2	3	0.68	0.001
	46 (C <sub>2</sub> NH <sub>6</sub> ) <sub>4</sub> Wl <sub>6</sub>	5	36	3	10	0.35	0.082
	47 (C <sub>2</sub> NH <sub>6</sub> ) <sub>4</sub> GeCl <sub>6</sub>	5	14	1	7	2.29	-0.002
	48 ((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>4</sub> BaBr <sub>6</sub>	13	29	2	7	2.95	0.004
	49 (CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )Nil <sub>3</sub>	9	12	3	4	1.30	0.025
	50 (C(NH <sub>2</sub> ) <sub>3</sub> )InI <sub>3</sub>	15	26	3	8	Metal	-0.008
	51 ((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> ) <sub>4</sub> PdI <sub>6</sub>	10	23	3	7	0.62	0.021
	52 ((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )MnBr <sub>3</sub>	8	9	2	4	0.93	0.057
	53 (C(NH <sub>2</sub> ) <sub>3</sub> ) <sub>4</sub> AsBr <sub>6</sub>	15	15	2	7	Failure	
	54 (CH(NH <sub>2</sub> ) <sub>2</sub> )GeI <sub>3</sub>	6	14	3	4	0.75	0.002

#	Chemical Formula	Decision Variables				Objective function Values	
		A	B	X	S	Obj_Eg	Obj_Ef
1	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )GeI <sub>3</sub>	8	14	3	2	1.18	0.001
2	(NH <sub>3</sub> NH <sub>2</sub> )CdCl <sub>3</sub>	3	25	1	8	1.32	-0.007
3	(C <sub>2</sub> NH <sub>6</sub> )ZnI <sub>3</sub>	5	13	3	6	1.07	0.005
4	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )AgI <sub>3</sub>	8	24	3	8	Metal	0.001
5	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )SmBr <sub>3</sub>	9	30	2	6	Metal	0.023
6	(C <sub>2</sub> OH <sub>5</sub> ) <sub>2</sub> ZnI <sub>6</sub>	7	13	3	7	1.58	0.006
7	(C <sub>4</sub> NH <sub>10</sub> )BaBr <sub>3</sub>	17	29	2	6	1.80	0.023
8	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> PtCl <sub>4</sub>	8	38	1	3	0.92	0.031
9	(C(NH <sub>2</sub> ) <sub>3</sub> ) <sub>4</sub> TmBr <sub>6</sub>	15	32	2	10	1.03	-0.031
10	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> SiI <sub>6</sub>	13	16	3	7	2.20	0.010
11	(CH(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> Zn <sub>2</sub> Br <sub>7</sub>	6	13	2	5	1.60	0.015
12	(C(NH <sub>2</sub> ) <sub>3</sub> )SnBr <sub>3</sub>	15	27	2	4	1.22	-0.043
13	((CH <sub>3</sub> ) <sub>3</sub> NH)SnBr <sub>3</sub>	14	27	2	8	1.22	-0.012
14	((CH <sub>3</sub> ) <sub>3</sub> NH) <sub>2</sub> GeBr <sub>4</sub>	14	14	2	3	1.29	0.000
15	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>4</sub> NbBr <sub>6</sub>	8	20	2	7	Metal	0.073
16	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )CdBr <sub>3</sub>	10	25	2	2	1.69	0.004
17	(NH <sub>3</sub> OH) <sub>4</sub> Pl <sub>6</sub>	4	4	3	10	0.20	0.089
18	(C <sub>5</sub> NH <sub>12</sub> ) <sub>2</sub> HfCl <sub>4</sub>	27	34	1	3	1.14	0.062
19	(C(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> )SmCl <sub>3</sub>	20	30	1	8	Metal	-0.074
20	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> CdBr <sub>4</sub>	11	25	2	3	1.84	-0.019
21	(CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> TmCl <sub>4</sub>	16	32	1	3	Metal	0.026
22	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> Ge <sub>2</sub> I <sub>7</sub>	8	14	3	5	0.55	0.015
23	(C(NH <sub>2</sub> ) <sub>3</sub> )PtCl <sub>3</sub>	15	38	1	8	0.27	0.015
24	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )AgI <sub>3</sub>	13	24	3	2	1.43	-0.006
25	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>4</sub> MoI <sub>4</sub>	8	21	3	3	Metal	0.146
26	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> Sb <sub>2</sub> Br <sub>7</sub>	13	28	2	5	Failure	Failure
27	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> GeBr <sub>4</sub>	13	14	2	3		
28	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> Cd <sub>2</sub> Br <sub>7</sub>	9	25	2	5		
29	(CH <sub>3</sub> (NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> BeI <sub>4</sub>	11	1	3	3		
30	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>4</sub> RhBr <sub>6</sub>	13	22	2	7		
31	(CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> BaBr <sub>3</sub>	16	29	2	2		
32	((CH <sub>3</sub> ) <sub>3</sub> NH <sub>2</sub> )BaBr <sub>3</sub>	10	29	2	2		
33	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )SnI <sub>3</sub>	9	27	3	1		
34	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )Nb <sub>4</sub> Br <sub>9</sub>	9	20	2	9		
35	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>4</sub> PtBr <sub>6</sub>	8	38	2	7		
36	(C <sub>3</sub> OH <sub>7</sub> )SnCl <sub>3</sub>	12	27	1	2		
37	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> Sn <sub>2</sub> Cl <sub>7</sub>	13	27	1	5		
38	(C <sub>3</sub> N <sub>2</sub> H <sub>5</sub> )YBr <sub>3</sub>	18	18	2	1	Metal	0.076
39	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )TmBr <sub>3</sub>	8	32	2	6	Metal	0.011
40	(C <sub>4</sub> NH <sub>10</sub> )YbCl <sub>3</sub>	21	33	1	6	3.41	0.016
41	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> ) <sub>4</sub> AgBr <sub>6</sub>	10	24	2	7	Metal	0.021
42	(C(NH <sub>2</sub> ) <sub>3</sub> )GeI <sub>3</sub>	15	14	3	2	0.95	-0.017
43	((CH <sub>3</sub> ) <sub>3</sub> NH)GeI <sub>3</sub>	14	14	3	6	0.66	-0.001
44	(NH <sub>3</sub> OH) <sub>2</sub> SiI <sub>4</sub>	4	3	3	3	0.76	0.076
45	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> GeI <sub>4</sub>	9	14	3	3	0.28	0.009
46	(NH <sub>3</sub> NH <sub>2</sub> ) <sub>4</sub> AsCl <sub>6</sub>	3	15	1	7	0.60	0.019
47	((CH <sub>3</sub> ) <sub>3</sub> NH)SnI <sub>3</sub>	14	27	3	8	0.67	-0.003
48	(C <sub>3</sub> OH <sub>7</sub> )TaBr <sub>3</sub>	12	35	2	4	1.05	0.112
49	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )SnI <sub>3</sub>	10	27	3	4	0.59	0.008
50	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> ) <sub>2</sub> SnBr <sub>4</sub>	10	27	2	3	0.70	-0.002
51	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> FeBr <sub>4</sub>	9	10	2	3	1.32	0.043
52	(NH <sub>3</sub> NH <sub>2</sub> )AsI <sub>9</sub>	3	15	3	9	0.98	0.084
53	(C <sub>4</sub> OH <sub>9</sub> ) <sub>2</sub> HfCl <sub>4</sub>	22	34	1	3	1.37	0.066
54	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )TiBr <sub>3</sub>	10	41	2	4	0.33	0.010

**Table S5.** The deserted entries (marked in red font) from all ‘A’-site molecule and ‘B’-site atom candidates, which were used for NSGA-II but not for the ensuing NSGA-III.

Deserted entries	
‘A’-site	‘B’-site
NH <sub>4</sub>	Be
CH <sub>3</sub> NH <sub>3</sub>	Mg
NH <sub>3</sub> NH <sub>2</sub>	Si
NH <sub>3</sub> OH	P
C <sub>2</sub> NH <sub>6</sub>	Ca
CH(NH <sub>2</sub> ) <sub>2</sub>	Sc
C <sub>2</sub> OH <sub>5</sub>	Ti
(CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub>	V
CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub>	Mn
(CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub>	Fe
CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub>	Co
C <sub>3</sub> OH <sub>7</sub>	Ni
(CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub>	Zn
(CH <sub>3</sub> ) <sub>3</sub> NH	Ge
C(NH <sub>2</sub> ) <sub>3</sub>	As
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>3</sub>	Sr
C <sub>4</sub> NH <sub>10</sub>	Cu
C <sub>3</sub> N <sub>2</sub> H <sub>5</sub>	Y
NC <sub>4</sub> H <sub>8</sub>	Zr
C(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>	Nb
C <sub>4</sub> NH <sub>10</sub>	Mo
C <sub>4</sub> OH <sub>9</sub>	Rh
(CH <sub>3</sub> ) <sub>4</sub> N	Pd
(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>2</sub> ) <sub>2</sub> NH <sub>2</sub>	Ag
CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> NH <sub>3</sub>	Cd
C <sub>3</sub> H <sub>4</sub> NS	In
C <sub>5</sub> NH <sub>12</sub>	Sn
C <sub>5</sub> OH <sub>11</sub>	Sb
C <sub>4</sub> H <sub>11</sub> N <sub>2</sub>	Ba
NH(CH <sub>2</sub> ) <sub>3</sub> S	Sm
C <sub>7</sub> H <sub>7</sub>	Eu
C(CH <sub>5</sub> )NH <sub>3</sub>	Tm
C <sub>6</sub> NH <sub>14</sub>	Yb
C <sub>6</sub> OH <sub>13</sub>	Hf
	Ta
	W
	Re
	Pt
	Au
	Hg
	Tl
	Bi

**Table S6.** The decision variable and objective function values for all the entries belonging to the 1<sup>st</sup> ~ 5<sup>th</sup> generations for NSGA-III.

#	Chemical Formula	Decision Variables							Objective function Values		
		A	B	X	S	θx	θy	θz	Obj_E <sub>g</sub>	Obj_E <sub>f</sub>	Obj_m <sub>e/h</sub> *
1 <sup>st</sup> Gen.	(C <sub>2</sub> OH <sub>10</sub> )SbI <sub>3</sub>	7	11	3	8	30	7	14	1.43	0.064	1.35
	(C <sub>4</sub> NH <sub>10</sub> )CdBr <sub>3</sub>	17	8	2	6	26	4	10	0.90	0.011	0.84
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )SiBr <sub>3</sub>	13	3	2	4	28	35	6		failure	
	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>4</sub> TmBr <sub>6</sub>	8	13	2	10	34	2	22	1.45	0.009	3.75
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>4</sub> GeI <sub>6</sub>	13	6	3	7	31	23	13	1.42	0.009	22.67
	((CH <sub>3</sub> ) <sub>3</sub> NH <sub>2</sub> ) <sub>2</sub> GeBr <sub>4</sub>	14	6	2	3	36	7	29	1.50	-0.012	9.80
	(NH <sub>3</sub> NH <sub>2</sub> ) <sub>2</sub> GeI <sub>4</sub>	3	6	3	3	13	1	33	0.42	0.008	0.27
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>4</sub> GeBr <sub>6</sub>	9	6	2	7	34	4	8	1.96	0.007	33.94
	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> SiI <sub>3</sub>	8	3	3	2	25	1	13	0.75	0.037	5.74
	((CH <sub>2</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> GeI <sub>4</sub>	10	6	3	3	8	34	10	0.21	0.005	0.66
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> GeBr <sub>3</sub>	13	6	2	1	10	26	23	1.39	-0.013	0.23
	(CH(NH <sub>2</sub> ) <sub>2</sub> )InI <sub>3</sub>	6	9	3	6	33	1	1	1.39	0.008	1.27
	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )AgBr <sub>3</sub>	8	7	2	1	18	32	29	Metal	0.025	-
	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )SnI <sub>3</sub>	10	10	3	4	19	33	19	0.40	-0.003	1.61
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> GeBr <sub>3</sub>	13	6	2	4	7	36	17	1.66	-0.004	6.78
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>3</sub> Ge <sub>2</sub> I <sub>7</sub>	9	6	3	5	5	35	22	0.22	0.001	3.03
	((CH <sub>3</sub> ) <sub>3</sub> NH)SnBr <sub>3</sub>	14	10	2	6	32	17	30	0.65	-0.016	0.33
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> InCl <sub>4</sub>	13	9	1	3	12	26	31	Metal	0.012	-
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>4</sub> HfCl <sub>6</sub>	13	15	1	7	34	4	20	1.44	0.020	33.68
	(C(NH <sub>2</sub> ) <sub>3</sub> )Sn <sub>2</sub> Br <sub>7</sub>	15	10	2	5	34	2	8	0.12	-0.039	0.36
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )InI <sub>3</sub>	11	9	3	1	11	36	25	Metal	0.001	-
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )InBr <sub>3</sub>	13	9	2	2	30	13	11	0.34	-0.003	1.63
	(C <sub>2</sub> OH <sub>5</sub> )GeBr <sub>3</sub>	7	6	2	4	3	36	19	0.74	-0.004	6.59
	(NC <sub>4</sub> H <sub>8</sub> ) <sub>4</sub> TmBr <sub>6</sub>	19	13	2	10	4	30	32	1.15	0.014	68.79
	(CH(NH <sub>2</sub> ) <sub>2</sub> )GeI <sub>3</sub>	6	6	3	8	24	31	10	0.47	0.004	1.66
	(C <sub>3</sub> OH <sub>7</sub> ) <sub>2</sub> Sb <sub>2</sub> Cl <sub>7</sub>	12	11	1	5	33	4	10	Metal	0.032	-
	(NH <sub>3</sub> NH <sub>2</sub> )GeI <sub>3</sub>	3	6	3	2	6	5	29	0.40	0.013	0.52
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> BiBr <sub>3</sub>	13	12	2	2	36	10	2	2.56	0.014	1.64
	(C <sub>4</sub> NH <sub>10</sub> )SbCl <sub>3</sub>	17	11	1	4	26	32	26	Metal	0.053	
	(NH <sub>3</sub> OH)GeI <sub>3</sub>	4	6	3	6	1	31	26	0.09	0.029	1.99
	(C(NH <sub>2</sub> ) <sub>3</sub> )SnI <sub>3</sub>	15	10	3	8	23	2	26	0.27	-0.014	1.65
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> InBr <sub>4</sub>	13	9	2	3	7	35	2	Metal	0.008	-
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )AgI <sub>3</sub>	13	7	3	2	17	25	25		failure	
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> SiCl <sub>4</sub>	11	3	1	3	19	17	31	1.39	0.017	3.25
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> CdBr <sub>4</sub>	11	8	2	3	1	25	29	1.12	-0.006	9.81
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> CdI <sub>4</sub>	9	8	3	3	5	17	16	0.36	0.138	7.74
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )GeI <sub>3</sub>	13	6	3	6	21	24	23	0.51	-0.00007	3.01
	(C <sub>2</sub> OH <sub>5</sub> ) <sub>3</sub> In <sub>2</sub> I <sub>7</sub>	7	9	3	5	35	2	2	Metal	0.016	-
	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )InCl <sub>3</sub>	10	9	1	8	35	15	8	1.27	0.009	8.08
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> SnBr <sub>6</sub>	13	10	2	10	32	1	9	1.79	0.001	12.60
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> YbCl <sub>3</sub>	13	14	1	6	32	6	23	3.25	0.017	18.25
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> Nil <sub>4</sub>	9	5	3	3	28	29	6	Metal	0.023	-
	(C <sub>3</sub> OH <sub>7</sub> )SbI <sub>3</sub>	12	11	3	6	34	2	13	1.06	0.041	12.97
	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )CdCl <sub>3</sub>	10	8	1	4	3	5	20	1.97	0.007	12.38
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )BaBr <sub>3</sub>	13	12	2	6	1	31	1	2.83	0.007	10.79
	(CH(NH <sub>2</sub> ) <sub>2</sub> )InBr <sub>3</sub>	6	9	2	6	5	36	24	0.48	-0.006	2.80
	(CH(NH <sub>2</sub> ) <sub>2</sub> ) <sub>4</sub> Tml <sub>6</sub>	6	13	3	7	34	3	30	0.66	0.009	150.00
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )GeBr <sub>3</sub>	9	6	2	8	3	35	20	1.28	-0.015	0.54
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )GeI <sub>3</sub>	9	6	3	6	35	4	34	0.26	0.001	1.25
	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )SnBr <sub>3</sub>	10	10	2	8	31	1	12	0.72	-0.010	0.962

#	Chemical Formula	Decision Variables						Objective function Values			
		A	B	X	S	$\theta_x$	$\theta_y$	$\theta_z$	Obj_Eg	Obj_Ef	Obj_m <sub>e/h</sub> *
1	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )SnCl <sub>3</sub>	8	10	1	6	21	4	22	1.24	-0.011	0.70
2	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>3</sub> Mn <sub>2</sub> I <sub>7</sub>	11	4	3	5	21	21	30	1.29	0.039	1.91
3	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )InCl <sub>3</sub>	8	9	1	2	20	22	29	1.04	-0.008	3.79
4	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )GeBr <sub>3</sub>	10	6	2	6	35	4	32	0.97	-0.017	2.94
5	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )InI <sub>3</sub>	11	9	3	6	3	34	21	1.18	-0.009	1.67
6	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )SbCl <sub>3</sub>	13	11	1	4	19	14	27		Failure	
7	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )SbBr <sub>3</sub>	13	11	2	4	31	6	4	Metal	0.018	-
8	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )Ge <sub>2</sub> I <sub>7</sub>	8	6	3	5	12	33	22	0.28	0.007	0.49
9	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )NiCl <sub>3</sub>	13	5	1	4	20	29	20		Failure	
10	(C <sub>2</sub> OH <sub>5</sub> ) <sub>3</sub> Ag <sub>2</sub> Br <sub>7</sub>	7	7	2	5	5	36	20	Metal	0.008	-
11	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )AgBr <sub>3</sub>	10	7	2	6	18	33	9	Metal	0.000	-
12	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )SnBr <sub>3</sub>	13	10	2	2	5	31	26	1.47	-0.009	6.45
13	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )In <sub>2</sub> Br <sub>7</sub>	8	9	2	5	25	15	26	0.44	0.006	48.08
14	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )TmCl <sub>3</sub>	13	13	1	6	27	16	24	Metal	0.019	-
15	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )InBr <sub>3</sub>	10	9	2	2	20	16	12	0.06	-0.001	3.08
16	(NH <sub>3</sub> OH)GeBr <sub>3</sub>	4	6	2	6	9	32	28	0.45	0.014	1.48
17	(C <sub>3</sub> OH <sub>7</sub> )SbBr <sub>3</sub>	12	11	2	6	29	4	12	1.31	0.001	6.85
18	(C <sub>2</sub> OH <sub>5</sub> ) <sub>2</sub> Ge <sub>2</sub> Br <sub>7</sub>	7	6	2	5	6	26	16	0.49	-0.011	0.77
19	(C <sub>2</sub> OH <sub>5</sub> ) <sub>2</sub> SnBr <sub>4</sub>	7	10	2	3	13	16	15	0.09	0.001	0.27
20	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> SnI <sub>4</sub>	8	10	3	3	21	11	23	0.09	0.003	2.84
21	(C <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> GeI <sub>4</sub>	5	6	3	3	10	31	27	0.14	0.004	0.81
22	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> ) <sub>2</sub> Ge <sub>2</sub> I <sub>7</sub>	10	6	3	5	7	28	16	0.04	0.003	0.79
23	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> SnBr <sub>4</sub>	11	10	2	3	1	36	10	0.38	-0.010	0.70
24	(C <sub>2</sub> OH <sub>5</sub> ) <sub>3</sub> Ge <sub>2</sub> I <sub>7</sub>	7	6	3	5	3	36	21	0.14	0.005	1.02
25	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> Ni <sub>2</sub> I <sub>7</sub>	9	5	3	5	28	29	6	Metal	0.029	-
26	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> SnCl <sub>6</sub>	13	10	1	7	35	9	10	1.91	-0.003	16.33
27	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>4</sub> SnBr <sub>6</sub>	9	10	2	10	33	1	16	1.74	0.009	11.60
28	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> Sn <sub>2</sub> I <sub>7</sub>	13	10	3	5	6	29	26	0.13	-0.002	4.48
29	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> CdI <sub>4</sub>	11	8	3	3	4	25	28	0.66	0.117	1.51
30	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )CdI <sub>3</sub>	11	8	3	4	1	31	9	0.50	0.232	0.96
31	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> SbBr <sub>4</sub>	11	11	2	3	1	31	12	Metal	0.006	-
32	(C <sub>3</sub> OH <sub>7</sub> ) <sub>3</sub> Sn <sub>2</sub> Br <sub>7</sub>	12	10	2	5	33	12	14	0.40	-0.009	0.21
33	(C <sub>3</sub> OH <sub>7</sub> )SnBr <sub>3</sub>	12	10	2	6	35	7	18	0.29	-0.010	2.25
34	(NH <sub>3</sub> OH)GeBr <sub>3</sub>	4	6	2	4	19	17	31	1.04	0.001	2.61
35	(C <sub>3</sub> OH <sub>7</sub> ) <sub>3</sub> Ge <sub>2</sub> I <sub>7</sub>	12	6	3	5	34	5	18	0.18	0.003	0.59
36	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )InI <sub>3</sub>	13	9	3	4	21	23	21		Failure	
37	(C <sub>3</sub> OH <sub>7</sub> )SnBr <sub>3</sub>	12	10	2	2	28	23	25	1.19	-0.007	2.69
38	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )InBr <sub>3</sub>	13	9	2	2	36	10	2	0.10	-0.004	2.74
39	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )SnCl <sub>3</sub>	11	10	1	6	33	9	9	1.02	-0.013	0.74
40	(C <sub>2</sub> OH <sub>5</sub> )GeI <sub>3</sub>	7	6	3	8	17	33	10	0.44	0.002	1.28
41	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> ) <sub>2</sub> InI <sub>4</sub>	10	9	3	3	25	21	25	Metal	0.011	-
42	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> Ge <sub>2</sub> Br <sub>7</sub>	8	6	2	5	9	23	25	0.71	-0.005	0.76
43	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> GeI <sub>4</sub>	9	6	3	3	28	31	9	0.22	0.002	0.49
44	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>4</sub> TmBr <sub>6</sub>	11	13	2	10	33	2	15	0.92	-0.013	80.41
45	(C <sub>2</sub> OH <sub>5</sub> )InBr <sub>3</sub>	7	9	2	4	35	3	12	0.61	0.017	10.66
46	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>4</sub> CdI <sub>6</sub>	8	8	3	7	34	24	15	1.20	0.080	1.40
47	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )GeBr <sub>3</sub>	10	6	2	8	4	35	19	1.39	-0.017	7.56
48	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )YbI <sub>6</sub>	10	14	3	7	28	30	11	2.23	0.008	7.49
49	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>4</sub> GeBr <sub>6</sub>	11	6	2	7	32	3	13	1.74	-0.001	9.25
50	(C <sub>2</sub> NH <sub>2</sub> )GeBr <sub>3</sub>	5	6	2	6	2	31	20	0.73	-0.022	1.72
51	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )AgBr <sub>3</sub>	13	7	2	2	14	25	26	1.40	0.006	5.93
52	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )AgI <sub>3</sub>	11	7	3	4	1	36	7	Metal	0.003	-
53	((CH <sub>3</sub> ) <sub>3</sub> NH <sub>2</sub> )Cd <sub>2</sub> Br <sub>7</sub>	10	8	2	5	25	16	9	0.82	0.012	10.26
54	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )SnCl <sub>3</sub>	13	10	1	6	33	10	8	1.53	-0.011	2.74

#	Chemical Formula	Decision Variables							Objective function Values		
		A	B	X	S	$\theta_X$	$\theta_Y$	$\theta_Z$	Obj_Eg	Obj_Ef	Obj_m <sub>e/h</sub> *
1	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>4</sub> CdCl <sub>6</sub>	9	8	1	7	14	21	16	2.16	0.013	52.30
2	(C <sub>2</sub> OH <sub>5</sub> ) <sub>2</sub> Gel <sub>4</sub>	7	6	3	3	7	31	26	0.17	0.004	0.55
3	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )CdCl <sub>3</sub>	9	8	1	6	21	4	29	1.06	0.008	6.13
4	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )InI <sub>3</sub>	9	9	3	1	5	17	14	Metal	0.012	-
5	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>3</sub> Ge <sub>2</sub> Br <sub>7</sub>	13	6	2	5	5	34	13	1.41	-0.007	12.99
6	(C <sub>2</sub> OH <sub>5</sub> )GeI <sub>3</sub>	7	6	3	4	25	2	13	0.40	0.010	0.60
7	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )SnI <sub>3</sub>	11	10	3	4	31	18	28	0.66	-0.022	1.29
8	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> ) <sub>3</sub> Ag <sub>2</sub> Br <sub>7</sub>	10	7	2	5	31	22	14	Metal	0.012	-
9	(C(NH <sub>2</sub> ) <sub>3</sub> ) <sub>3</sub> SnCl <sub>6</sub>	15	10	1	7	34	6	10	2.22	0.389	108.75
10	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )GeI <sub>3</sub>	11	6	3	4	9	13	18	0.87	0.324	2.74
11	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>3</sub> Sn <sub>2</sub> Br <sub>7</sub>	11	10	2	5	28	3	15	0.22	-0.014	4.06
12	(C <sub>2</sub> OH <sub>5</sub> ) <sub>3</sub> Ge <sub>2</sub> I <sub>7</sub>	7	6	3	5	5	17	16	0.25	-0.0003	0.57
13	(C <sub>3</sub> OH <sub>7</sub> ) <sub>3</sub> In <sub>2</sub> Br <sub>7</sub>	12	9	2	5	9	24	2	1.24	0.007	15.43
14	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )SnBr <sub>3</sub>	13	10	2	4	9	20	13	1.40	-0.004	22.39
15	(C <sub>3</sub> OH <sub>7</sub> )SnBr <sub>3</sub>	12	10	2	4	24	11	23	1.01	-0.00036	0.93
16	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>3</sub> Ge <sub>2</sub> I <sub>7</sub>	8	6	3	5	20	22	26	0.15	0.008	0.65
17	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>3</sub> Ag <sub>2</sub> Br <sub>7</sub>	11	7	2	5	17	32	22	Metal	0.020	-
18	(C <sub>2</sub> OH <sub>5</sub> )InCl <sub>3</sub>	7	9	1	6	24	3	7	0.32	-0.002	1.99
19	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>4</sub> InBr <sub>6</sub>	11	9	2	10	33	1	7	0.21	0.002	14.05
20	(C <sub>2</sub> NH <sub>6</sub> ) <sub>3</sub> Ag <sub>2</sub> Br <sub>7</sub>	5	7	2	5	23	25	27	Metal	0.007	-
21	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> CdBr <sub>4</sub>	8	8	2	3	28	28	24	0.48	0.007	1.62
22	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )GeI <sub>3</sub>	11	6	3	6	9	18	25	0.38	-0.013	0.54
23	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )SnBr <sub>3</sub>	11	10	2	8	34	4	19	0.94	-0.017	0.73
24	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )CdBr <sub>3</sub>	9	8	2	6	35	4	25	0.91	0.004	1.33
25	(C <sub>2</sub> OH <sub>5</sub> )GeI <sub>3</sub>	7	6	3	6	29	20	5	0.14	0.002	0.28
26	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )TmBr <sub>3</sub>	11	13	2	8	32	23	12	Metal	-0.013	-
27	(C <sub>2</sub> OH <sub>5</sub> )InBr <sub>3</sub>	7	9	2	6	12	33	24	0.55	-0.001	6.16
28	(C <sub>2</sub> OH <sub>5</sub> )GeCl <sub>3</sub>	7	6	1	4	23	15	33	1.83	-0.014	3.43
29	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )InCl <sub>6</sub>	9	9	1	7	10	13	12	0.84	0.009	9.39
30	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>3</sub> Sn <sub>2</sub> Br <sub>7</sub>	13	10	2	5	35	5	8	0.45	-0.0004	1.37
31	(C <sub>2</sub> OH <sub>5</sub> )AgBr <sub>3</sub>	7	7	2	4	24	20	22	1.44	0.009	7.95
32	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )SnBr <sub>3</sub>	8	10	2	8	17	14	9	1.01	-0.009	2.18
33	(NH <sub>3</sub> OH) <sub>2</sub> GeI <sub>4</sub>	4	6	3	3	13	12	21	0.43	0.035	0.24
34	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> GeI <sub>4</sub>	13	6	3	3	32	16	18	0.51	0.003	11.57
35	((CH <sub>3</sub> ) <sub>2</sub> NH)SnCl <sub>3</sub>	14	10	1	6	31	11	29	1.24	-0.018	3.31
36	(C <sub>2</sub> OH <sub>5</sub> )SiI <sub>3</sub>	7	3	3	8	17	33	10	0.22	0.045	1.11
37	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )GeBr <sub>3</sub>	8	6	2	6	5	33	13	1.02	-0.013	8.89
38	(C <sub>3</sub> OH <sub>7</sub> )InI <sub>3</sub>	12	9	3	4	23	19	18	0.32	0.008	5.83
39	(C <sub>2</sub> OH <sub>5</sub> )SnI <sub>3</sub>	7	10	3	6	30	2	16	0.24	-0.003	0.28
40	(C <sub>2</sub> OH <sub>5</sub> ) <sub>2</sub> AgBr <sub>4</sub>	7	7	2	3	11	13	9	Metal	0.004	-
41	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>3</sub> Yb <sub>2</sub> Cl <sub>7</sub>	13	14	1	5	29	11	22	3.62	0.016	5.90
42	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )GeI <sub>3</sub>	10	6	3	6	35	4	32	0.31	-0.005	0.51
43	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )SbBr <sub>3</sub>	11	11	2	6	25	15	13	1.17	-0.007	1.94
44	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )SbCl <sub>3</sub>	11	11	1	6	26	13	21	0.79	-0.002	4.95
45	(C <sub>2</sub> OH <sub>5</sub> ) <sub>2</sub> Sn <sub>2</sub> I <sub>7</sub>	12	10	3	5	18	13	19	0.51	-0.003	0.58
46	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> ) <sub>4</sub> InI <sub>6</sub>	10	9	3	7	17	27	21	0.50	0.009	9.29
47	(NH <sub>3</sub> NH <sub>2</sub> ) <sub>2</sub> CdI <sub>4</sub>	3	8	3	3	13	1	33	Failure		
48	(NH <sub>3</sub> NH <sub>2</sub> ) <sub>2</sub> GeI <sub>4</sub>	3	6	3	3	19	1	33	0.34	0.011	0.23
49	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> InI <sub>4</sub>	9	9	3	3	7	30	20	Metal	0.014	-
50	(CH(NH <sub>2</sub> ) <sub>2</sub> )InI <sub>3</sub>	6	9	3	4	33	1	1	1.19	0.026	3.54
51	(C <sub>2</sub> OH <sub>5</sub> )SnBr <sub>3</sub>	7	10	2	2	18	22	23	1.31	-0.006	2.26
52	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )Tm <sub>4</sub> Br <sub>9</sub>	11	13	2	9	33	2	15	Metal	-0.054	-
53	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )InI <sub>3</sub>	11	9	3	6	32	21	22	1.04	-0.010	3.61
54	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )InCl <sub>3</sub>	9	9	1	6	22	25	10	0.26	-0.004	6.79

#	Chemical Formula	Decision Variables							Objective function Values		
		A	B	X	S	$\theta_x$	$\theta_y$	$\theta_z$	$Obj\_E_g$	$Obj\_E_f$	$Obj\_m_{e/h}^*$
1	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )InI <sub>3</sub>	13	9	3	6	34	3	9	0.79	0.006	1.18
2	(C <sub>2</sub> OH <sub>5</sub> )GeI <sub>3</sub>	7	6	3	4	33	2	27	0.59	0.006	1.68
3	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )AgI <sub>3</sub>	10	7	3	4	22	35	22	1.29	0.019	9.02
4	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )GeI <sub>3</sub>	9	6	3	6	4	29	16	0.33	0.0003	0.84
5	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )TmBr <sub>3</sub>	13	13	2	2	36	10	2	Metal	-0.019	-
6	(C <sub>2</sub> NH <sub>6</sub> )InI <sub>3</sub>	5	9	3	6	33	1	1	1.42	-0.004	5.54
7	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )GeI <sub>3</sub>	10	6	3	1	1	36	18	0.10	-0.030	0.24
8	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )CdCl <sub>3</sub>	11	8	1	4	18	13	25	2.05	-0.014	2.86
9	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )SnI <sub>3</sub>	9	10	3	2	23	14	29	0.72	-0.010	1.74
10	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )AgBr <sub>3</sub>	13	7	2	2	15	25	25	1.39	0.007	6.38
11	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )SnCl <sub>3</sub>	11	10	1	4	21	13	24	1.66	-0.009	8.94
12	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>3</sub> Sn <sub>2</sub> I <sub>7</sub>	9	10	3	5	17	29	13	0.86	0.001	0.08
13	(C <sub>2</sub> NH <sub>6</sub> )GeBr <sub>3</sub>	5	6	2	4	5	26	17	1.47	-0.007	5.27
14	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )SbI <sub>3</sub>	13	11	3	6	8	27	23	1.48	0.049	2.74
15	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )SnI <sub>3</sub>	13	10	3	8	18	23	21	0.50	-0.006	0.41
16	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )SnI <sub>3</sub>	11	10	3	1	19	35	25	0.42	-0.015	0.07
17	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>3</sub> Cd <sub>2</sub> Br <sub>7</sub>	13	8	2	5	33	22	21	1.42	0.003	5.23
18	(C(NH <sub>2</sub> ) <sub>3</sub> )GeI <sub>3</sub>	15	6	3	8	23	2	26	0.65	-0.007	1.90
19	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )GeI <sub>3</sub>	11	6	3	4	7	34	20	0.65	-0.012	1.95
20	(NH <sub>3</sub> OH) <sub>2</sub> GeI <sub>4</sub>	4	6	3	3	18	16	31	0.43	0.032	0.25
21	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )GeI <sub>3</sub>	10	6	3	2	14	32	22	0.62	-0.002	0.65
22	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )SnBr <sub>3</sub>	8	10	2	6	34	5	10	0.50	-0.007	1.08
23	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )GeI <sub>3</sub>	10	6	3	4	20	4	24	0.92	0.011	6.19
24	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> CdI <sub>4</sub>	11	8	3	3	11	22	18	0.71	0.128	3.61
25	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>3</sub> In <sub>2</sub> I <sub>7</sub>	9	9	3	5	4	22	21	Metal	0.012	-
26	(CH(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> AgBr <sub>4</sub>	6	7	2	3	33	2	10	Metal	0.005	-
27	(C(NH <sub>2</sub> ) <sub>3</sub> )Sn <sub>2</sub> Br <sub>7</sub>	15	10	2	5	34	2	6	0.31	-0.044	0.26
4 <sup>th</sup> Gen.	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )Ba <sub>2</sub> Cl <sub>7</sub>	13	12	1	5	32	12	20	Failure		
	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )Ge <sub>2</sub> Br <sub>7</sub>	10	6	2	5	13	11	17	0.79	-0.007	0.54
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )CdBr <sub>3</sub>	13	8	2	2	18	19	8	1.65	0.006	6.78
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )AgI <sub>3</sub>	13	7	3	2	16	25	26	Failure		
	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )GeBr <sub>3</sub>	8	6	2	2	17	18	31	1.96	-0.018	8.15
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>3</sub> Sn <sub>2</sub> Br <sub>7</sub>	9	10	2	5	13	16	18	0.27	-0.008	1.14
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )AgI <sub>3</sub>	9	7	3	4	26	33	21	1.49	0.018	8.74
	(C(NH <sub>2</sub> ) <sub>3</sub> ) <sub>4</sub> SnBr <sub>6</sub>	15	10	2	7	28	17	18	1.76	-0.035	2.50
	(C <sub>3</sub> OH <sub>7</sub> )SnI <sub>3</sub>	12	10	3	6	24	30	25	0.37	-0.011	1.86
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )GeI <sub>4</sub>	9	6	3	3	20	29	16	0.14	0.008	1.87
	(C <sub>2</sub> NH <sub>6</sub> ) <sub>2</sub> CdBr <sub>4</sub>	5	8	2	3	35	1	22	1.30	-0.004	18.97
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )GeCl <sub>3</sub>	13	6	1	6	24	19	9	2.10	-0.026	3.35
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )GeBr <sub>3</sub>	13	6	2	6	9	20	22	1.21	-0.012	4.17
	(NH <sub>3</sub> OH) <sub>2</sub> GeBr <sub>4</sub>	4	6	2	3	19	17	31	0.11	0.013	0.33
	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )CdBr <sub>3</sub>	10	8	2	6	11	8	22	0.82	0.004	0.76
	((CH <sub>3</sub> ) <sub>3</sub> NH)GeBr <sub>3</sub>	14	6	2	6	32	17	30	1.27	-0.019	1.51
	((CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub> )SnCl <sub>3</sub>	10	10	1	6	33	10	8	1.14	-0.015	2.00
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> GeBr <sub>4</sub>	9	6	2	3	13	29	19	0.59	-0.005	3.44
	(C <sub>2</sub> NH <sub>6</sub> ) <sub>2</sub> CdI <sub>4</sub>	5	8	3	3	20	11	21	0.11	0.166	2.03
	(NH <sub>3</sub> OH) <sub>2</sub> GeI <sub>4</sub>	4	6	3	3	10	12	21	0.44	0.029	0.98
	(NC <sub>4</sub> H <sub>8</sub> ) <sub>2</sub> SnCl <sub>4</sub>	19	10	1	3	34	6	29	0.48	-0.005	8.70
	(C <sub>2</sub> OH <sub>5</sub> ) <sub>3</sub> Ge <sub>2</sub> I <sub>7</sub>	7	6	3	5	8	17	16	0.08	0.004	3.34
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )GeI <sub>3</sub>	11	6	3	6	9	18	24	0.41	-0.014	2.08
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )SnI <sub>3</sub>	8	10	3	6	31	9	26	0.09	0.002	1.38
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )InBr <sub>3</sub>	9	9	2	4	18	18	24	0.14	0.007	5.38
	(C <sub>2</sub> OH <sub>5</sub> ) <sub>3</sub> Sn <sub>2</sub> I <sub>7</sub>	7	10	3	5	32	3	10	0.93	-0.003	0.23
	(C <sub>3</sub> OH <sub>7</sub> ) <sub>4</sub> SnBr <sub>6</sub>	12	10	2	7	35	7	18	1.29	0.005	9.23

#	Chemical Formula	Decision Variables							Objective function Values		
		A	B	X	S	$\theta_x$	$\theta_y$	$\theta_z$	Obj_Eg	Obj_Ef	Obj_m <sub>e/h</sub> *
5 <sup>th</sup> Gen.	(CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> CdI <sub>3</sub>	13	8	3	2	34	16	20	0.82	0.204	3.54
	((CH <sub>2</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> GeI <sub>4</sub>	10	6	3	3	1	25	17	0.31	0.004	0.62
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )SnI <sub>3</sub>	9	10	3	6	17	29	13	0.30	-0.005	114.26
	(C <sub>2</sub> NH <sub>6</sub> ) <sub>2</sub> AgBr <sub>4</sub>	5	7	2	3	25	5	15	Metal	0.008	-
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> SnBr <sub>4</sub>	13	10	2	3	16	12	27	0.48	-0.004	0.86
	(C <sub>3</sub> O <sub>H</sub> ) <sub>2</sub> CdBr <sub>4</sub>	12	8	2	3	22	23	22	1.37	0.006	9.14
	(C(NH <sub>2</sub> ) <sub>3</sub> )SbBr <sub>3</sub>	15	11	2	6	20	15	19	1.18	-0.043	0.20
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> GeBr <sub>3</sub>	13	6	2	6	4	34	4	1.31	-0.014	0.56
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> SnCl <sub>4</sub>	13	10	1	3	19	15	26	1.35	-0.007	24.52
	(C <sub>2</sub> OH) <sub>5</sub> SnI <sub>3</sub>	7	10	3	6	32	3	10	0.23	-0.004	0.45
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>4</sub> Nil <sub>6</sub>	13	5	3	7	30	2	12	1.00	0.016	72.31
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )InI <sub>3</sub>	11	9	3	2	12	25	28	0.75	-0.011	2.54
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>3</sub> Cd <sub>2</sub> I <sub>7</sub>	11	8	3	5	5	32	9	0.54	0.165	2.85
	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>3</sub> Ge <sub>2</sub> I <sub>7</sub>	8	6	3	5	17	8	21	0.18	0.011	0.66
	(C <sub>2</sub> OH) <sub>5</sub> GeI <sub>4</sub>	7	6	3	3	24	28	13	0.08	0.001	0.92
	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> )GeI <sub>3</sub>	8	6	3	4	11	16	26	0.79	0.021	3.18
	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> GeBr <sub>3</sub>	10	6	2	2	14	21	18	1.65	-0.015	2.66
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )InBr <sub>3</sub>	11	9	2	2	36	17	16	0.04	-0.007	2.66
	((CH <sub>2</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> SnI <sub>4</sub>	10	10	3	3	20	33	14	0.34	-0.003	1.56
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> SiBr <sub>4</sub>	13	3	2	3	28	35	6	1.38	0.012	1.85
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )CdBr <sub>4</sub>	13	8	2	3	12	21	24	1.89	-0.004	0.89
	(C <sub>2</sub> NH <sub>6</sub> )GeI <sub>3</sub>	5	6	3	2	18	37	29	0.51	-0.002	1.67
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> Sn <sub>2</sub> I <sub>7</sub>	9	10	3	5	7	35	2	0.48	-0.004	0.29
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>3</sub> Ge <sub>2</sub> I <sub>7</sub>	11	6	3	5	27	20	17	0.19	-0.006	1.29
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> )Nil <sub>3</sub>	9	5	3	1	24	29	20	Metal	0.023	-
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )GeI <sub>3</sub>	13	6	3	8	18	17	16	0.84	0.003	4.69
	(NH <sub>3</sub> NH <sub>2</sub> )GeI <sub>3</sub>	3	6	3	2	13	1	33	0.52	0.008	1.59
	(NH <sub>3</sub> OH)GeI <sub>3</sub>	4	6	3	4	12	23	30	0.41	0.015	1.02
	(C <sub>3</sub> O <sub>H</sub> ) <sub>2</sub> GeBr <sub>3</sub>	12	6	2	4	31	15	26	1.18	-0.006	11.76
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )GeI <sub>3</sub>	11	6	3	2	22	29	17	0.80	-0.011	4.72
	(C <sub>2</sub> OH) <sub>5</sub> <sub>2</sub> GeBr <sub>4</sub>	7	6	2	3	20	8	27	0.75	-0.010	0.87
	(NH <sub>3</sub> OH) <sub>2</sub> SnI <sub>4</sub>	4	10	3	3	13	22	25	0.66	0.029	0.17
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>3</sub> Ge <sub>2</sub> Br <sub>7</sub>	9	6	2	5	10	29	12	0.48	-0.004	1.56
	(C <sub>2</sub> OH) <sub>5</sub> <sub>3</sub> Ge <sub>2</sub> I <sub>7</sub>	7	6	3	5	16	18	30	0.06	0.003	1.84
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )GeI <sub>3</sub>	13	6	3	4	36	3	1	0.40	0.013	3.21
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>3</sub> Ge <sub>2</sub> Br <sub>7</sub>	9	6	2	5	9	16	11	0.68	-0.011	1.25
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> ) <sub>2</sub> SbBr <sub>6</sub>	13	11	2	7	2	35	27	0.46	0.006	20.95
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )GeCl <sub>3</sub>	13	6	1	6	23	19	9	2.10	-0.024	2.26
	(CH <sub>3</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> SnI <sub>4</sub>	9	10	3	3	5	17	16	0.20	-0.002	0.52
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> SnI <sub>4</sub>	11	10	3	3	18	19	9	0.06	-0.015	0.82
	(C <sub>3</sub> OH) <sub>7</sub> SnI <sub>3</sub>	12	10	3	6	18	5	22	0.20	-0.010	0.36
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )AgCl <sub>3</sub>	11	7	1	4	1	15	20	1.32	-0.016	1.40
	((CH <sub>3</sub> ) <sub>2</sub> CHNH <sub>3</sub> )SnBr <sub>3</sub>	13	10	2	4	32	2	14	1.29	-0.002	8.10
	((CH <sub>3</sub> ) <sub>3</sub> NH)GeCl <sub>3</sub>	14	6	1	6	24	19	9	2.03	-0.028	5.72
	((CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ) <sub>3</sub> Ge <sub>2</sub> Br <sub>7</sub>	8	6	2	5	9	23	26	0.54	-0.004	1.26
	(C <sub>2</sub> OH) <sub>5</sub> <sub>2</sub> GeI <sub>4</sub>	7	6	3	3	5	28	17	0.15	0.005	0.47
	(C(NH <sub>2</sub> ) <sub>3</sub> )SnI <sub>3</sub>	15	10	3	8	25	2	26	0.28	-0.009	1.79
	(C <sub>2</sub> OH) <sub>5</sub> <sub>3</sub> Ag <sub>2</sub> Br <sub>7</sub>	7	7	2	5	22	14	10	Metal	0.009	-
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> SnBr <sub>4</sub>	11	10	2	3	24	18	21	0.75	-0.016	2.16
	(C <sub>2</sub> OH) <sub>5</sub> GeCl <sub>3</sub>	7	6	1	4	6	24	3	1.81	-0.014	23.45
	((CH <sub>3</sub> ) <sub>3</sub> NH)SnI <sub>3</sub>	14	10	3	4	30	18	25	0.47	0.004	7.44
	(C <sub>2</sub> OH) <sub>5</sub> SnI <sub>3</sub>	7	10	3	6	21	9	17	0.36	-0.005	2.36
	((CH <sub>2</sub> ) <sub>2</sub> NH <sub>2</sub> )AgI <sub>3</sub>	10	7	3	2	6	35	20	Metal	0.009	-
	(CH <sub>3</sub> C(NH <sub>2</sub> ) <sub>2</sub> )AgBr <sub>3</sub>	11	7	2	6	35	11	5	1.51	-0.007	4.21