

补充材料

面向软晶格筛选的立方钙钛矿体模量可解释性描述符研究

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支撑材料中包含四个附表: 表 S1 汇总了由 Magpie 工具生成的 22 项元素特征, 包括英文名称、符号及中文名称; 表 S2 提供了 SISSO 模型所用的 213 个钙钛矿样本的元素特征数值、基于热-结构耦合描述符预测的体模量以及对应的 DFT 计算值; 表 S3 对应 VS-SISSO 模型, 列出了同一组钙钛矿样本的元素特征值、DFT 模量以及利用电子-热-结构三重耦合描述符预测的体模量; 表 S4 为预测数据集: 包含 169 种无铅钙钛矿候选材料, 这些材料的体模量预测值位于 10–20 GPa 范围内, 与 Pb-I 钙钛矿相近, 并给出了其元素特征值。

表 S1 magpie 生成 22 元素特征

Table S1. The 22 elemental features generated using Magpie

Elemental features	元素属性	Feature symbol
Number	原子序数	N
AtomicWeight	原子质量	AW
Column	原子所在元素周期表列数	C
CovalentRadius	原子共价半径	CR
NUnfilled	轨道上未填满的价电子总数	NU
NpUnfilled	p 轨道未填满的电子数	NpU
NfUnfilled	f 轨道未填满的电子数	NfU
NdUnfilled	d 轨道未填满的电子数	NdU
NdValence	d 价轨道被填满的电子数	NdV
GSmagmom	T=0K 基态下每个原子的 DFT 磁矩	GSm
SpaceGroupNumber	T=0K 基态结构的空群	SGN
MendelevNumber	门捷列夫数	MN
MeltingT	单质熔点	MT
Row	原子所在元素周期表的行数	R
Electronegativity	电负性	E
NsUnfilled	s 价轨道被填满的电子数	NsU
NValence	轨道上被填满的价电子总数	NV
NsValence	s 价轨道被填满的电子数	NsV
NpValence	p 价轨道被填满的电子数	NpV
NfValence	f 价轨道被填满的电子数	NfV

GSvolume_pa	T=0K 基态的高斯体积	GSV
GSbandgap	T=0K 基态的 DFT 带隙能	GSB

表 S2 SISSO 数据集: 213 个钙钛矿样本的元素特征及体模量 (预测值与 DFT 计算值)

Table S2. SISSO dataset: elemental features of 213 perovskite samples with bulk modulus (predicted and DFT-calculated values).

Formula	BM-DFT	BM-SISSO	meanMT	maxCR	meanGSV	ranCR	minN
Cs ₂ AgSbI ₆	17.62	14.91	506.29	244	53.75	105	47
Ba ₂ SbVO ₆	114.06	147.33	541.55	215	22.63	149	8
Rb ₂ AgBiCl ₆	23.96	21.76	343.38	220	37.77	118	17
Rb ₂ AgSbBr ₆	21.59	18.90	435.84	220	40.62	100	35
K ₂ RbBiCl ₆	14.38	18.42	255.95	220	41.68	118	17
Rb ₂ TlSbBr ₆	10.05	16.62	370.05	220	41.67	100	35
K ₂ KSbI ₆	9.91	13.46	423.44	203	50.89	64	19
BaTiSe ₃	60.87	60.73	884.6	215	31.60	95	22
CaHfO ₃	174.92	160.85	757.08	176	17.45	110	8
Cs ₂ TlSbBr ₆	14.36	16.47	367.87	244	46.68	124	35
K ₂ RbBiBr ₆	11.87	15.63	312.47	220	44.67	100	19
SrTiSe ₃	62.25	62.44	894.6	195	29.73	75	22
CaTiS ₃	78.56	75.06	844.21	176	26.36	71	16
Ba ₂ SbNbS ₆	61.76	62.99	798.39	215	33.16	110	16
K ₂ CuBiCl ₆	29.46	24.06	360.48	203	33.72	101	17
Ba ₂ BiVO ₆	129.02	137.93	505.62	215	22.77	149	8
Cs ₂ AgSbBr ₆	20.90	18.65	433.66	244	45.63	124	35
KSnI ₃	15.33	16.08	400.43	203	47.08	64	19
K ₂ NaSbI ₆	11.96	17.89	426.88	203	46.51	64	11
Cs ₂ TlSbCl ₆	17.25	19.21	311.35	244	43.69	142	17
Sr ₂ BiVSe ₆	51.61	56.21	779.14	195	30.99	75	23
Ba ₂ BiNbO ₆	125.72	127.74	562.32	215	23.29	149	8
K ₂ RbSbI ₆	9.38	12.90	421.04	220	52.65	81	19
Cs ₂ RbSbBr ₆	12.39	15.70	341.42	244	53.06	124	35
Rb ₂ CuBiCl ₆	28.81	17.03	355.66	220	37.24	118	17
Sr ₂ BiVS ₆	62.38	66.00	715.75	195	30.91	90	16
SrZrS ₃	73.03	65.63	868.61	195	30.95	90	16
CsPbCl ₃	22.68	19.20	283.4	244	43.47	142	17
SrHfSe ₃	65.44	57.83	1007.6	195	30.83	75	34
SrTiS ₃	76.85	73.33	831.21	195	29.65	90	16
BaHfO ₃	164.31	143.10	734.08	215	22.62	149	8
Cs ₂ KBiI ₆	9.49	12.90	380.52	244	59.56	105	19
Rb ₂ KSbCl ₆	15.43	19.91	289.48	220	43.30	118	17
K ₂ AgBiI ₆	17.91	14.77	477.34	203	45.35	64	19
Cs ₂ NaSbCl ₆	12.74	26.48	290.74	244	43.93	142	11
K ₂ CuBiBr ₆	25.08	19.93	417.00	203	36.71	83	19
Sr ₂ BiNbO ₆	130.06	132.81	572.32	195	21.42	129	8

Cs ₂ KSbI ₆	9.63	13.15	416.45	244	59.42	105	19
BaZrSe ₃	59.70	55.26	922	215	32.90	95	34
Rb ₂ CuSbI ₆	20.21	15.95	520.75	220	48.21	88	29
Cs ₂ CuSbI ₆	19.82	15.91	518.58	244	53.22	112	29
Rb ₂ CuSbBr ₆	25.14	19.07	448.12	220	40.09	100	29
CaHfSe ₃	66.37	58.44	1020.6	176	27.54	56	20
K ₂ KBiI ₆	9.72	13.16	387.50	203	51.03	64	19
K ₂ KSbBr ₆	12.79	16.75	350.81	203	42.77	83	19
Rb ₂ KSbBr ₆	12.69	16.63	346.00	220	46.29	100	19
KPbI ₃	15.18	13.42	419.53	203	46.05	64	19
Cs ₂ RbSbI ₆	9.10	12.70	414.05	244	61.19	105	37
CsSnF ₃	44.64	42.06	193.43	244	35.63	187	9
Ca ₂ SbVO ₆	124.35	152.85	564.55	176	17.47	110	8
K ₂ KBiBr ₆	12.49	16.23	314.87	203	42.91	83	19
K ₂ CuSbCl ₆	30.09	24.88	396.42	203	33.58	101	17
Cs ₂ AgBiI ₆	17.29	14.56	470.36	244	53.89	105	47
K ₂ RbBiI ₆	9.21	12.64	385.10	220	52.79	81	19
BaTiO ₃	167.56	165.10	621.08	215	21.51	149	8
Ba ₂ SbNbSe ₆	51.69	54.21	861.77	215	33.24	95	34
Cs ₂ AgBiCl ₆	23.06	21.44	341.21	244	42.77	142	17
CaZrS ₃	73.87	66.67	881.61	176	27.66	71	16
K ₂ TlSbI ₆	12.07	13.56	447.49	203	46.27	64	19
K ₂ RbSbBr ₆	12.11	16.05	348.41	220	44.53	100	19
SrHfO ₃	171.16	152.45	744.08	195	20.74	129	8
RbSnI ₃	15.53	13.86	395.61	220	50.61	81	37
Ca ₂ BiNbSe ₆	52.88	54.00	848.84	176	28.21	56	20
Ca ₂ BiVS ₆	63.30	67.13	728.75	176	27.62	71	16
RbPbCl ₃	22.77	19.41	285.57	220	38.46	118	17
SrTiO ₃	176.58	165.02	631.08	195	19.64	129	8
Rb ₂ CuBiBr ₆	24.66	19.72	412.18	220	40.23	100	29
Ca ₂ SbTaSe ₆	54.63	56.26	938.77	176	28.07	56	20
K ₂ TlBiI ₆	11.77	13.26	411.55	203	46.41	64	19
KSnBr ₃	19.61	17.32	327.80	203	38.96	83	19
SrZrSe ₃	60.43	56.32	932	195	31.03	75	34
K ₂ AgSbBr ₆	22.03	19.07	440.65	203	37.09	83	19
Rb ₂ KBiI ₆	9.67	14.87	382.69	220	54.55	81	19
K ₂ TlBiBr ₆	15.14	16.24	338.92	203	38.29	83	19
Rb ₂ NaBiI ₆	11.59	14.98	386.12	220	50.17	81	11
K ₂ CuSbBr ₆	25.57	20.57	452.94	203	36.57	83	19
RbSnBr ₃	19.57	17.21	322.98	220	42.48	100	35
Cs ₂ TlBiCl ₆	16.32	18.71	275.41	244	43.83	142	17
Rb ₂ RbSbBr ₆	11.92	15.92	343.59	220	48.06	100	35
Rb ₂ RbBiI ₆	9.06	12.58	380.28	220	56.32	81	37
Ba ₂ BiTaO ₆	129.53	127.19	616.32	215	23.28	149	8

KPbCl ₃	22.83	39.45	290.38	203	34.94	101	17
Ca ₂ BiTaS ₆	65.34	63.02	839.45	176	28.13	71	16
Ca ₂ BiVO ₆	138.40	151.45	528.62	176	17.61	110	8
Cs ₂ KBiBr ₆	12.13	16.01	307.89	244	51.44	124	19
Ca ₂ SbNbO ₆	152.23	145.29	621.25	176	17.99	110	8
Cs ₂ KSbBr ₆	12.36	16.35	343.82	244	51.30	124	19
BaHfSe ₃	64.54	56.52	997.6	215	32.71	95	34
K ₂ AgSbI ₆	18.28	15.13	513.28	203	45.21	64	19
BaZrS ₃	72.20	64.14	858.61	215	32.82	110	16
Rb ₂ NaSbBr ₆	14.92	21.16	349.43	220	41.91	100	11
CaZrSe ₃	61.18	57.12	945	176	27.74	56	20
Ca ₂ SbTaS ₆	65.31	65.99	875.39	176	27.99	71	16
Rb ₂ CuBiI ₆	19.87	15.61	484.81	220	48.35	88	29
Cs ₂ NaBiI ₆	35.89	16.76	383.95	244	55.18	105	11
BaZrO ₃	147.87	139.38	658.48	215	22.82	149	8
Sr ₂ BiTaSe ₆	53.45	53.40	889.84	195	31.50	75	34
KPbF ₃	43.72	40.44	219.52	203	26.06	146	9
K ₂ KBiCl ₆	14.77	19.52	258.35	203	39.92	101	17
Sr ₂ BiVO ₆	135.06	145.53	515.62	195	20.90	129	8
BaHfS ₃	78.84	65.62	934.21	215	32.63	110	16
Rb ₂ NaSbI ₆	11.78	17.78	422.06	220	50.03	81	11
KSnCl ₃	23.06	20.42	271.28	203	35.97	101	17
Rb ₂ NaBiCl ₆	17.70	23.75	256.97	220	39.06	118	11
Cs ₂ RbSbCl ₆	14.14	18.61	284.90	244	50.07	142	17
Rb ₂ AgBiBr ₆	21.18	18.32	399.90	220	40.76	100	35
Sr ₂ BiTaS ₆	64.61	62.03	826.45	195	31.42	90	16
Ca ₂ SbTaO ₆	143.55	144.06	675.25	176	17.98	110	8
Ca ₂ BiVSe ₆	52.53	57.22	792.14	176	27.70	56	20
RbPbF ₃	42.27	40.48	214.71	220	29.59	163	9
Cs ₂ TlSbI ₆	11.72	13.40	440.50	244	54.80	105	51
SrHfS ₃	79.95	67.17	944.21	195	30.75	90	16
RbPbBr ₃	19.18	16.51	342.09	220	41.45	100	35
Rb ₂ TlBiCl ₆	16.71	18.96	277.59	220	38.82	118	17
K ₂ AgSbCl ₆	25.02	22.75	384.13	203	34.10	101	17
Cs ₂ RbBiI ₆	8.95	12.40	378.11	244	61.32	105	37
Ca ₂ BiNbS ₆	63.22	62.98	785.45	176	28.13	71	16
Ba ₂ BiTaS ₆	63.62	60.76	816.45	215	33.29	110	16
K ₂ RbSbCl ₆	14.71	19.11	291.89	220	41.54	118	17
RbPbI ₃	15.16	13.33	414.72	220	49.57	81	37
CsPbBr ₃	19.11	16.41	339.92	244	46.46	124	35
Cs ₂ RbBiCl ₆	13.85	18.10	248.96	244	50.21	142	17
Ca ₂ SbNbS ₆	62.14	66.22	821.39	176	28.00	71	16
Rb ₂ RbBiBr ₆	11.66	15.56	307.65	220	48.19	100	35
CsSnI ₃	15.51	13.74	393.44	244	55.61	105	50

$\text{Sr}_2\text{SbNbO}_6$	136.28	140.48	608.25	195	21.28	129	8
$\text{Cs}_2\text{CuBiBr}_6$	23.96	19.42	410.01	244	45.24	124	29
$\text{Ba}_2\text{SbTaSe}_6$	52.98	54.21	915.77	215	33.23	95	34
$\text{Rb}_2\text{TlBiBr}_6$	14.38	16.21	334.11	220	41.81	100	35
Ca_2SbVS_6	61.80	70.69	764.69	176	27.48	71	16
$\text{Sr}_2\text{SbVSe}_6$	52.57	58.62	815.07	195	30.85	75	23
$\text{Cs}_2\text{NaSbBr}_6$	14.27	21.96	347.26	244	46.92	124	11
$\text{Cs}_2\text{CuSbCl}_6$	28.16	23.88	389.43	244	42.11	142	17
$\text{Rb}_2\text{RbBiCl}_6$	14.04	18.33	251.13	220	45.21	118	17
RbSnF_3	40.95	42.83	195.60	220	30.62	163	9
$\text{Ca}_2\text{BiTaO}_6$	137.70	135.15	639.32	176	18.12	110	8
$\text{Ba}_2\text{BiNbSe}_6$	51.16	52.27	825.84	215	33.38	95	34
$\text{Sr}_2\text{SbTaO}_6$	135.50	139.40	662.25	195	21.27	129	8
$\text{Cs}_2\text{KBiCl}_6$	14.61	18.96	251.37	244	48.45	142	17
KSnF_3	43.55	42.73	200.42	203	27.10	146	9
K_2KSbCl_6	16.70	20.11	294.29	203	39.78	101	17
CaZrO_3	157.52	153.94	681.48	176	17.65	110	8
$\text{Cs}_2\text{NaBiCl}_6$	47.55	25.65	254.80	244	44.07	142	11
$\text{Sr}_2\text{SbTaSe}_6$	53.90	55.33	925.77	195	31.36	75	34
$\text{Sr}_2\text{SbTaS}_6$	64.67	64.78	862.39	195	31.28	90	16
$\text{Rb}_2\text{NaBiBr}_6$	14.70	20.72	313.49	220	42.05	100	11
BaTiS_3	75.06	70.91	821.21	215	31.52	110	16
$\text{Rb}_2\text{AgBiI}_6$	17.69	14.69	472.53	220	48.88	81	37
$\text{Ca}_2\text{SbNbSe}_6$	52.98	56.35	884.77	176	28.08	56	20
KPbBr_3	19.23	16.58	346.90	203	37.93	83	19
$\text{Cs}_2\text{KSbCl}_6$	14.90	19.46	287.30	244	48.31	142	17
$\text{Rb}_2\text{RbSbI}_6$	9.27	12.86	416.22	220	56.18	81	37
$\text{Rb}_2\text{KBiBr}_6$	12.45	16.17	310.06	220	46.43	100	19
$\text{Rb}_2\text{AgSbI}_6$	18.03	15.06	508.47	220	48.74	81	37
$\text{Rb}_2\text{AgSbCl}_6$	24.44	22.45	379.32	220	37.63	118	17
$\text{Rb}_2\text{NaSbCl}_6$	18.05	24.32	292.91	220	38.92	118	11
$\text{K}_2\text{TlSbBr}_6$	14.88	16.69	374.86	203	38.15	83	19
$\text{K}_2\text{NaSbCl}_6$	18.57	24.59	297.73	203	35.40	101	11
$\text{Cs}_2\text{TlBiBr}_6$	14.07	16.04	331.93	244	46.82	124	35
$\text{K}_2\text{AgBiBr}_6$	21.56	18.50	404.71	203	37.23	83	19
$\text{Ba}_2\text{BiTaSe}_6$	52.56	52.43	879.84	215	33.37	95	34
CaTiSe_3	63.72	63.75	907.6	176	26.44	56	20
$\text{Ba}_2\text{SbTaS}_6$	63.73	68.20	852.39	215	33.15	110	16
$\text{Cs}_2\text{RbBiBr}_6$	11.51	15.40	305.48	244	53.20	124	35
$\text{Rb}_2\text{KBiCl}_6$	15.10	19.27	253.54	220	43.44	118	17
CsPbI_3	15.09	13.23	412.55	244	54.58	105	53
$\text{K}_2\text{TlSbCl}_6$	17.32	19.77	318.34	203	35.16	101	17
Ba_2SbVS_6	60.16	66.84	741.69	215	32.64	110	16
$\text{Rb}_2\text{CuSbCl}_6$	29.44	24.46	391.60	220	37.10	118	17

Cs ₂ NaBiBr ₆	75.84	21.38	311.32	244	47.06	124	11
Rb ₂ TlSbI ₆	11.94	13.49	442.68	220	49.80	81	37
Rb ₂ KSbI ₆	9.87	13.24	418.63	220	54.42	81	19
Rb ₂ TlSbCl ₆	17.06	19.57	313.53	220	38.69	118	17
Ca ₂ BiNbO ₆	133.55	135.99	585.32	176	18.13	110	8
K ₂ NaBiBr ₆	15.04	20.81	318.31	203	38.52	83	11
K ₂ NaBiI ₆	11.75	17.52	390.94	203	46.64	64	11
Cs ₂ NaSbI ₆	12.76	17.22	419.89	244	55.04	105	11
Ba ₂ BiNbS ₆	61.65	60.63	762.45	215	33.30	110	16
CsSnCl ₃	22.90	20.03	264.29	244	44.50	142	17
CaHfS ₃	81.06	68.25	957.21	176	27.46	71	16
K ₂ CuSbI ₆	20.41	16.07	525.57	203	44.69	71	19
Sr ₂ SbNbS ₆	62.11	64.97	808.39	195	31.29	90	16
CaTiO ₃	171.91	171.56	644.08	176	16.35	110	8
Cs ₂ AgBiBr ₆	20.54	18.18	397.73	244	45.76	124	35
Rb ₂ RbSbCl ₆	14.42	18.89	287.07	220	45.07	118	17
Ba ₂ SbNbO ₆	127.14	133.42	598.25	215	23.15	149	8
K ₂ CuBiI ₆	20.13	15.70	489.63	203	44.83	71	19
Sr ₂ BiNbS ₆	62.55	61.93	772.45	195	31.43	90	16
Cs ₂ AgSbCl ₆	23.41	22.07	377.14	244	42.64	142	17
SrZrO ₃	153.34	147.55	668.48	195	20.94	129	8
Cs ₂ CuBiI ₆	19.52	15.36	482.64	244	53.36	112	29
Sr ₂ SbVO ₆	87.47	80.01	551.55	195	20.76	129	8
RbSnCl ₃	23.00	20.33	266.46	220	39.5	118	17
CsSnBr ₃	19.50	17.09	320.81	244	47.49	124	35
Ba ₂ BiVSe ₆	50.60	54.9	769.14	215	32.86	95	23
K ₂ NaSbBr ₆	15.26	21.35	354.25	203	38.38	83	11
Ba ₂ SbTaO ₆	130.54	133.01	652.25	215	23.14	149	8
Rb ₂ TlBiI ₆	11.67	13.18	406.74	220	49.93	81	37
Ba ₂ SbVSe ₆	51.39	56.78	805.07	215	32.72	95	23
Cs ₂ CuBiCl ₆	27.63	23.25	353.49	244	42.25	142	17
Sr ₂ BiNbSe ₆	51.97	53.21	835.84	195	31.51	75	34
Cs ₂ CuSbBr ₆	24.37	20.00	445.95	244	45.10	124	29
K ₂ NaBiCl ₆	17.96	23.94	261.79	203	35.53	101	11
Ca ₂ SbVSe ₆	53.49	59.64	828.07	176	27.56	56	20
Sr ₂ SbNbSe ₆	52.48	55.48	871.77	195	31.37	75	34
Ba ₂ BiVS ₆	61.11	64.25	705.75	215	32.78	110	16
Ca ₂ BiTaSe ₆	54.15	54.14	902.84	176	28.21	56	20
CsPbF ₃	41.25	39.93	212.54	244	34.59	187	9
K ₂ TlBiCl ₆	16.93	19.09	282.40	203	35.30	101	17
Cs ₂ TlBiI ₆	11.47	13.08	404.56	244	54.94	105	53
Sr ₂ SbVS ₆	61.83	69.05	751.69	195	30.77	90	16
Sr ₂ BiTaO ₆	134.23	132.12	626.32	195	21.41	129	8
K ₂ AgBiCl ₆	24.49	22.03	348.19	203	34.24	101	17

表 S3 VS-SISSO 数据集：同一组 213 个钙钛矿样本的元素特征及体模量（VS-SISSO 预测值与 DFT 计算值）

Table S3. VS-SISSO dataset: elemental features of the same 213 perovskite samples with bulk modulus (VS-SISSO predicted and DFT-calculated values).

Formula	BM-DFT	BM-VS	meanE	n _B	n _X	minCR	meanMT	maxNpU
Cs ₂ AgSbI ₆	17.62	16.38	2.15	2	-1	139	506.29	3
Ba ₂ SbVO ₆	114.06	126.04	2.61	4	-2	66	541.55	3
Rb ₂ AgBiCl ₆	23.96	25.72	2.45	2	-1	102	343.38	3
Rb ₂ AgSbBr ₆	21.59	21.83	2.33	2	-1	120	435.84	3
K ₂ RbBiCl ₆	14.38	19.42	2.34	2	-1	102	255.95	3
Rb ₂ TlSbBr ₆	10.05	13.98	2.30	2	-1	120	370.05	5
K ₂ KSbI ₆	9.91	12.88	2.04	2	-1	139	423.44	3
BaTiSe ₃	60.87	62.85	2.01	4	-2	120	884.6	2
CaHfO ₃	174.92	172.07	2.52	4	-2	66	757.08	2
Cs ₂ TlSbBr ₆	14.36	13.84	2.30	2	-1	120	367.87	5
K ₂ RbBiBr ₆	11.87	15.81	2.22	2	-1	120	312.47	3
SrTiSe ₃	62.25	64.02	2.02	4	-2	120	894.6	2
CaTiS ₃	78.56	73.61	2.05	4	-2	105	844.21	2
Ba ₂ SbNbS ₆	61.76	59.76	2.09	4	-2	105	798.39	3
K ₂ CuBiCl ₆	29.46	26.38	2.45	2	-1	102	360.48	3
Ba ₂ BiVO ₆	129.02	121.37	2.60	4	-2	66	505.62	3
Cs ₂ AgSbBr ₆	20.90	21.63	2.33	2	-1	120	433.66	3
KSnI ₃	15.33	11.72	2.15	2	-1	139	400.43	4
K ₂ NaSbI ₆	11.96	13.13	2.05	2	-1	139	426.88	3
Cs ₂ TlSbCl ₆	17.25	17.35	2.42	2	-1	102	311.35	5
Sr ₂ BiVSe ₆	51.61	50.81	2.08	4	-2	120	779.14	3
Ba ₂ BiNbO ₆	125.72	127.90	2.60	4	-2	66	562.32	3
K ₂ RbSbI ₆	9.38	12.84	2.04	2	-1	139	421.04	3
Cs ₂ RbSbBr ₆	12.39	16.65	2.22	2	-1	120	341.42	3
Rb ₂ CuBiCl ₆	28.81	26.17	2.45	2	-1	102	355.66	3
Sr ₂ BiVS ₆	62.38	57.07	2.10	4	-2	105	715.75	3
SrZrS ₃	73.03	70.79	2.00	4	-2	105	868.61	2
CsPbCl ₃	22.68	20.66	2.52	2	-1	102	283.4	4
SrHfSe ₃	65.44	64.81	1.98	4	-2	120	1007.6	2
SrTiS ₃	76.85	72.26	2.04	4	-2	105	831.21	2
BaHfO ₃	164.31	166.37	2.50	4	-2	66	734.08	2
Cs ₂ KBiI ₆	9.49	11.87	2.03	2	-1	139	380.52	3
Rb ₂ KSbCl ₆	15.43	20.96	2.34	2	-1	102	289.48	3
K ₂ AgBiI ₆	17.91	15.85	2.15	2	-1	139	477.34	3
Cs ₂ NaSbCl ₆	12.74	21.12	2.35	2	-1	102	290.74	3
K ₂ CuBiBr ₆	25.08	21.14	2.33	2	-1	120	417.00	3
Sr ₂ BiNbO ₆	130.06	130.30	2.61	4	-2	66	572.32	3

Cs ₂ KSbI ₆	9.63	12.65	2.04	2	-1	139	416.45	3
BaZrSe ₃	59.70	61.43	1.97	4	-2	120	922	2
Rb ₂ CuSbI ₆	20.21	17.82	2.15	2	-1	132	520.75	3
Cs ₂ CuSbI ₆	19.82	17.66	2.14	2	-1	132	518.58	3
Rb ₂ CuSbBr ₆	25.14	22.12	2.33	2	-1	120	448.12	3
CaHfSe ₃	66.37	65.96	1.99	4	-2	120	1020.6	2
K ₂ KBiI ₆	9.72	12.11	2.04	2	-1	139	387.50	3
K ₂ KSbBr ₆	12.79	17.04	2.22	2	-1	120	350.81	3
Rb ₂ KSbBr ₆	12.69	16.90	2.22	2	-1	120	346.00	3
KPbI ₃	15.18	13.21	2.22	2	-1	139	419.53	4
Cs ₂ RbSbI ₆	9.10	12.60	2.04	2	-1	139	414.05	3
CsSnF ₃	44.64	45.44	2.93	2	-1	57	193.43	4
Ca ₂ SbVO ₆	124.35	131.02	2.63	4	-2	66	564.55	3
K ₂ KBiBr ₆	12.49	15.89	2.22	2	-1	120	314.87	3
K ₂ CuSbCl ₆	30.09	27.93	2.45	2	-1	102	396.42	3
Cs ₂ AgBiI ₆	17.29	15.60	2.14	2	-1	139	470.36	3
K ₂ RbBiI ₆	9.21	12.06	2.04	2	-1	139	385.10	3
BaTiO ₃	167.56	158.79	2.55	4	-2	66	621.08	2
Ba ₂ SbNbSe ₆	51.69	52.98	2.07	4	-2	120	861.77	3
Cs ₂ AgBiCl ₆	23.06	25.48	2.44	2	-1	102	341.21	3
CaZrS ₃	73.87	72.10	2.01	4	-2	105	881.61	2
K ₂ TlSbI ₆	12.07	10.53	2.12	2	-1	139	447.49	5
K ₂ RbSbBr ₆	12.11	16.97	2.22	2	-1	120	348.41	3
SrHfO ₃	171.16	169.17	2.51	4	-2	66	744.08	2
RbSnI ₃	15.53	11.63	2.15	2	-1	139	395.61	4
Ca ₂ BiNbSe ₆	52.88	53.59	2.09	4	-2	120	848.84	3
Ca ₂ BiVS ₆	63.30	58.20	2.11	4	-2	105	728.75	3
RbPbCl ₃	22.77	20.87	2.52	2	-1	102	285.57	4
SrTiO ₃	176.58	161.64	2.56	4	-2	66	631.08	2
Rb ₂ CuBiBr ₆	24.66	20.99	2.33	2	-1	120	412.18	3
Ca ₂ SbTaSe ₆	54.63	56.15	2.08	4	-2	120	938.77	3
K ₂ TlBiI ₆	11.77	9.90	2.12	2	-1	139	411.55	5
KSnBr ₃	19.61	15.33	2.33	2	-1	120	327.80	4
SrZrSe ₃	60.43	62.59	1.98	4	-2	120	932	2
K ₂ AgSbBr ₆	22.03	21.97	2.33	2	-1	120	440.65	3
Rb ₂ KBiI ₆	9.67	12.01	2.04	2	-1	139	382.69	3
K ₂ TlBiBr ₆	15.14	13.17	2.30	2	-1	120	338.92	5
Rb ₂ NaBiI ₆	11.59	12.25	2.05	2	-1	139	386.12	3
K ₂ CuSbBr ₆	25.57	22.26	2.33	2	-1	120	452.94	3
RbSnBr ₃	19.57	15.18	2.33	2	-1	120	322.98	4
Cs ₂ TlBiCl ₆	16.32	16.04	2.41	2	-1	102	275.41	5
Rb ₂ RbSbBr ₆	11.92	16.83	2.22	2	-1	120	343.59	3
Rb ₂ RbBiI ₆	9.06	11.96	2.04	2	-1	139	380.28	3
Ba ₂ BiTaO ₆	129.53	133.03	2.59	4	-2	66	616.32	3

KPbCl ₃	22.83	21.08	2.52	2	-1	102	290.38	4
Ca ₂ BiTaS ₆	65.34	61.94	2.1	4	-2	105	839.45	3
Ca ₂ BiVO ₆	138.40	126.36	2.62	4	-2	66	528.62	3
Cs ₂ KBiBr ₆	12.13	15.56	2.21	2	-1	120	307.89	3
Ca ₂ SbNbO ₆	152.23	137.31	2.62	4	-2	66	621.25	3
Cs ₂ KSbBr ₆	12.36	16.72	2.22	2	-1	120	343.82	3
BaHfSe ₃	64.54	63.65	1.96	4	-2	120	997.6	2
K ₂ AgSbI ₆	18.28	16.64	2.15	2	-1	139	513.28	3
BaZrS ₃	72.20	69.47	1.99	4	-2	105	858.61	2
Rb ₂ NaSbBr ₆	14.92	17.21	2.23	2	-1	120	349.43	3
CaZrSe ₃	61.18	63.73	1.99	4	-2	120	945	2
Ca ₂ SbTaS ₆	65.31	63.52	2.10	4	-2	105	875.39	3
Rb ₂ CuBiI ₆	19.87	17.00	2.15	2	-1	132	484.81	3
Cs ₂ NaBiI ₆	35.89	12.11	2.04	2	-1	139	383.95	3
BaZrO ₃	147.87	158.14	2.50	4	-2	66	658.48	2
Sr ₂ BiTaSe ₆	53.45	53.84	2.07	4	-2	120	889.84	3
KPbF ₃	43.72	51.57	3.01	2	-1	57	219.52	4
K ₂ KBiCl ₆	14.77	19.52	2.34	2	-1	102	258.35	3
Sr ₂ BiVO ₆	135.06	123.77	2.61	4	-2	66	515.62	3
BaHfS ₃	78.84	72.18	1.98	4	-2	105	934.21	2
Rb ₂ NaSbI ₆	11.78	13.04	2.05	2	-1	139	422.06	3
KSnCl ₃	23.06	18.85	2.45	2	-1	102	271.28	4
Rb ₂ NaBiCl ₆	17.70	19.68	2.35	2	-1	102	256.97	3
Cs ₂ RbSbCl ₆	14.14	20.64	2.34	2	-1	102	284.90	3
Rb ₂ AgBiBr ₆	21.18	20.68	2.33	2	-1	120	399.90	3
Sr ₂ BiTaS ₆	64.61	60.80	2.09	4	-2	105	826.45	3
Ca ₂ SbTaO ₆	143.55	142.20	2.61	4	-2	66	675.25	3
Ca ₂ BiVSe ₆	52.53	51.79	2.09	4	-2	120	792.14	3
RbPbF ₃	42.27	50.95	3.01	2	-1	57	214.71	4
Cs ₂ TlSbI ₆	11.72	10.34	2.12	2	-1	139	440.50	5
SrHfS ₃	79.95	73.51	1.99	4	-2	105	944.21	2
RbPbBr ₃	19.18	17.01	2.40	2	-1	120	342.09	4
Rb ₂ TlBiCl ₆	16.71	16.21	2.42	2	-1	102	277.59	5
K ₂ AgSbCl ₆	25.02	27.51	2.45	2	-1	102	384.13	3
Cs ₂ RbBiI ₆	8.95	11.82	2.03	2	-1	139	378.11	3
Ca ₂ BiNbS ₆	63.22	60.39	2.11	4	-2	105	785.45	3
Ba ₂ BiTaS ₆	63.62	59.67	2.07	4	-2	105	816.45	3
K ₂ RbSbCl ₆	14.71	21.06	2.34	2	-1	102	291.89	3
RbPbI ₃	15.16	13.11	2.22	2	-1	139	414.72	4
CsPbBr ₃	19.11	16.84	2.4	2	-1	120	339.92	4
Cs ₂ RbBiCl ₆	13.85	18.98	2.33	2	-1	102	248.96	3
Ca ₂ SbNbS ₆	62.14	62.03	2.11	4	-2	105	821.39	3
Rb ₂ RbBiBr ₆	11.66	15.66	2.22	2	-1	120	307.65	3
CsSnI ₃	15.51	11.50	2.14	2	-1	139	393.44	4

Sr ₂ SbNbO ₆	136.28	134.76	2.61	4	-2	66	608.25	3
Cs ₂ CuBiBr ₆	23.96	20.80	2.32	2	-1	120	410.01	3
Ba ₂ SbTaSe ₆	52.98	54.17	2.06	4	-2	120	915.77	3
Rb ₂ TlBiBr ₆	14.38	13.05	2.30	2	-1	120	334.11	5
Ca ₂ SbVS ₆	61.80	59.90	2.11	4	-2	105	764.69	3
Sr ₂ SbVSe ₆	52.57	52.22	2.08	4	-2	120	815.07	3
Cs ₂ NaSbBr ₆	14.27	17.03	2.23	2	-1	120	347.26	3
Cs ₂ CuSbCl ₆	28.16	27.49	2.44	2	-1	102	389.43	3
Rb ₂ RbBiCl ₆	14.04	19.19	2.34	2	-1	102	251.13	3
RbSnF ₃	40.95	45.92	2.94	2	-1	57	195.60	4
Ca ₂ BiTaO ₆	137.70	137.94	2.61	4	-2	66	639.32	3
Ba ₂ BiNbSe ₆	51.16	51.62	2.07	4	-2	120	825.84	3
Sr ₂ SbTaO ₆	135.50	139.69	2.60	4	-2	66	662.25	3
Cs ₂ KBiCl ₆	14.61	19.09	2.33	2	-1	102	251.37	3
KSnF ₃	43.55	46.53	2.94	2	-1	57	200.42	4
K ₂ KSbCl ₆	16.70	21.16	2.34	2	-1	102	294.29	3
CaZrO ₃	157.52	163.85	2.53	4	-2	66	681.48	2
Cs ₂ NaBiCl ₆	47.55	19.46	2.34	2	-1	102	254.80	3
Sr ₂ SbTaSe ₆	53.90	55.16	2.07	4	-2	120	925.77	3
Sr ₂ SbTaS ₆	64.67	62.38	2.09	4	-2	105	862.39	3
Rb ₂ NaBiBr ₆	14.70	16.04	2.23	2	-1	120	313.49	3
BaTiS ₃	75.06	70.92	2.03	4	-2	105	821.21	2
Rb ₂ AgBiI ₆	17.69	15.75	2.15	2	-1	139	472.53	3
Ca ₂ SbNbSe ₆	52.98	54.96	2.09	4	-2	120	884.77	3
KPbBr ₃	19.23	17.15	2.40	2	-1	120	346.90	4
Cs ₂ KSbCl ₆	14.90	20.74	2.34	2	-1	102	287.30	3
Rb ₂ RbSbI ₆	9.27	12.74	2.04	2	-1	139	416.22	3
Rb ₂ KBiBr ₆	12.45	15.74	2.22	2	-1	120	310.06	3
Rb ₂ AgSbI ₆	18.03	16.54	2.15	2	-1	139	508.47	3
Rb ₂ AgSbCl ₆	24.44	27.31	2.45	2	-1	102	379.32	3
Rb ₂ NaSbCl ₆	18.05	21.34	2.35	2	-1	102	292.91	3
K ₂ TlSbBr ₆	14.88	14.10	2.30	2	-1	120	374.86	5
K ₂ NaSbCl ₆	18.57	21.55	2.35	2	-1	102	297.73	3
Cs ₂ TlBiBr ₆	14.07	12.90	2.29	2	-1	120	331.93	5
K ₂ AgBiBr ₆	21.56	20.83	2.33	2	-1	120	404.71	3
Ba ₂ BiTaSe ₆	52.56	52.85	2.06	4	-2	120	879.84	3
CaTiSe ₃	63.72	65.19	2.03	4	-2	120	907.6	2
Ba ₂ SbTaS ₆	63.73	61.25	2.08	4	-2	105	852.39	3
Cs ₂ RbBiBr ₆	11.51	15.49	2.21	2	-1	120	305.48	3
Rb ₂ KBiCl ₆	15.10	19.31	2.34	2	-1	102	253.54	3
CsPbI ₃	15.09	12.97	2.22	2	-1	139	412.55	4
K ₂ TlSbCl ₆	17.32	17.69	2.42	2	-1	102	318.34	5
Ba ₂ SbVS ₆	60.16	57.63	2.09	4	-2	105	741.69	3
Rb ₂ CuSbCl ₆	29.44	27.73	2.45	2	-1	102	391.60	3

Cs ₂ NaBiBr ₆	75.84	15.87	2.22	2	-1	120	311.32	3
Rb ₂ TlSbI ₆	11.94	10.45	2.12	2	-1	139	442.68	5
Rb ₂ KSbI ₆	9.87	12.79	2.04	2	-1	139	418.63	3
Rb ₂ TlSbCl ₆	17.06	17.53	2.42	2	-1	102	313.53	5
Ca ₂ BiNbO ₆	133.55	132.85	2.62	4	-2	66	585.32	3
K ₂ NaBiBr ₆	15.04	16.19	2.23	2	-1	120	318.31	3
K ₂ NaBiI ₆	11.75	12.35	2.05	2	-1	139	390.94	3
Cs ₂ NaSbI ₆	12.76	12.90	2.05	2	-1	139	419.89	3
Ba ₂ BiNbS ₆	61.65	58.13	2.08	4	-2	105	762.45	3
CsSnCl ₃	22.90	18.44	2.44	2	-1	102	264.29	4
CaHfS ₃	81.06	74.82	2.00	4	-2	105	957.21	2
K ₂ CuSbI ₆	20.41	17.92	2.15	2	-1	132	525.57	3
Sr ₂ SbNbS ₆	62.11	60.89	2.10	4	-2	105	808.39	3
CaTiO ₃	171.91	164.64	2.57	4	-2	66	644.08	2
Cs ₂ AgBiBr ₆	20.54	20.49	2.32	2	-1	120	397.73	3
Rb ₂ RbSbCl ₆	14.42	20.85	2.34	2	-1	102	287.07	3
Ba ₂ SbNbO ₆	127.14	132.36	2.60	4	-2	66	598.25	3
K ₂ CuBiI ₆	20.13	17.10	2.15	2	-1	132	489.63	3
Sr ₂ BiNbS ₆	62.55	59.25	2.1	4	-2	105	772.45	3
Cs ₂ AgSbCl ₆	23.41	27.07	2.45	2	-1	102	377.14	3
SrZrO ₃	153.34	160.93	2.52	4	-2	66	668.48	2
Cs ₂ CuBiI ₆	19.52	16.84	2.14	2	-1	132	482.64	3
Sr ₂ SbVO ₆	87.47	128.45	2.62	4	-2	66	551.55	3
RbSnCl ₃	23.00	18.64	2.45	2	-1	102	266.46	4
CsSnBr ₃	19.50	15.02	2.32	2	-1	120	320.81	4
Ba ₂ BiVSe ₆	50.60	49.83	2.07	4	-2	120	769.14	3
K ₂ NaSbBr ₆	15.26	17.35	2.23	2	-1	120	354.25	3
Ba ₂ SbTaO ₆	130.54	137.29	2.59	4	-2	66	652.25	3
Rb ₂ TlBiI ₆	11.67	9.82	2.12	2	-1	139	406.74	5
Ba ₂ SbVSe ₆	51.39	51.23	2.07	4	-2	120	805.07	3
Cs ₂ CuBiCl ₆	27.63	25.94	2.44	2	-1	102	353.49	3
Sr ₂ BiNbSe ₆	51.97	52.60	2.08	4	-2	120	835.84	3
Cs ₂ CuSbBr ₆	24.37	21.92	2.32	2	-1	120	445.95	3
K ₂ NaBiCl ₆	17.96	19.90	2.35	2	-1	102	261.79	3
Ca ₂ SbVSe ₆	53.49	53.21	2.09	4	-2	120	828.07	3
Sr ₂ SbNbSe ₆	52.48	53.97	2.08	4	-2	120	871.77	3
Ba ₂ BiVS ₆	61.11	55.95	2.09	4	-2	105	705.75	3
Ca ₂ BiTaSe ₆	54.15	54.82	2.08	4	-2	120	902.84	3
CsPbF ₃	41.25	50.46	3.01	2	-1	57	212.54	4
K ₂ TlBiCl ₆	16.93	16.39	2.42	2	-1	102	282.40	5
Cs ₂ TlBiI ₆	11.47	9.71	2.11	2	-1	139	404.56	5
Sr ₂ SbVS ₆	61.83	58.76	2.10	4	-2	105	751.69	3
Sr ₂ BiTaO ₆	134.23	135.41	2.60	4	-2	66	626.32	3
K ₂ AgBiCl ₆	24.49	25.93	2.45	2	-1	102	348.19	3

表 4 预测数据集: 169 种无铅钙钛矿候选材料的元素特征与体模量预测值 (10–20 GPa, 接近 CsPbI₃)Table S4. Predicted dataset: elemental features and bulk modulus (10 – 20 GPa) of 169 lead-free perovskite candidate materials similar to CsPbI₃.

Formula	BM-SISSO	minN	meanMT	maxCR	ranCR
Cs ₂ HgSbBr ₆	16.02	35	333.60	244	124
Cs ₂ LiInBr ₆	19.83	3	308.14	244	124
Na ₂ GaHgCl ₆	17.98	11	230.85	166	64
Rb ₂ NaSbBr ₆	19.66	11	349.43	220	100
Na ₂ InHgBr ₆	16.04	11	300.06	166	46
Cs ₂ RbAsBr ₆	15.73	33	360.04	244	125
Cs ₂ NaInBr ₆	17.34	11	299.86	244	124
Cs ₂ RbBiBr ₆	12.32	35	305.48	244	124
K ₂ TlInCl ₆	19.37	17	270.94	203	101
Cs ₂ KEuCl ₆	19.66	17	306.43	244	142
Cs ₂ NaGaBr ₆	16.72	11	287.17	244	124
Cs ₂ RbEuCl ₆	18.72	17	304.02	244	142
K ₂ RbBiCl ₆	16.47	17	255.95	220	118
Cs ₂ GaHgBr ₆	13.52	31	273.52	244	124
Rb ₂ TlInBr ₆	15.19	35	322.64	220	100
Cs ₂ KAsBr ₆	18.43	19	362.45	244	125
K ₂ RbPrBr ₆	18.59	19	378.43	220	100
K ₂ RbNdBr ₆	19.13	19	387.43	220	100
Rb ₂ NaInBr ₆	16.99	11	302.03	220	100
K ₂ GaHgBr ₆	14.59	19	280.50	203	83
Cs ₂ RbAuBr ₆	16.76	35	384.77	244	124
K ₂ RbGaCl ₆	15.28	17	231.80	220	118
Cs ₂ RbLaCl ₆	19.38	17	313.82	244	142
Na ₂ GaHgBr ₆	15.60	11	287.37	166	46
Cs ₂ TlBiCl ₆	19.67	17	275.41	244	142
Cs ₂ NaBiBr ₆	17.72	11	311.32	244	124
K ₂ TlGaCl ₆	18.67	17	258.25	203	101
K ₂ HgSbBr ₆	17.57	19	340.59	203	83
Cs ₂ InBiBr ₆	15.09	35	317.21	244	124
K ₂ TlInBr ₆	17.08	19	327.46	203	83
K ₂ GaHgCl ₆	15.95	17	223.98	203	101
Rb ₂ InBiCl ₆	18.56	17	262.86	220	118
Rb ₂ InHgBr ₆	13.37	35	288.37	220	100
Rb ₂ NaBiBr ₆	17.31	11	313.49	220	100
Cs ₂ TlHgBr ₆	14.37	35	300.93	244	124
K ₂ SBrCl ₆	16.45	16	235.68	203	101
Cs ₂ KInCl ₆	15.28	17	239.90	244	142
K ₂ NaSbBr ₆	19.42	11	354.25	203	83

Rb ₂ GaAgBr ₆	19.52	31	375.75	220	100
Cs ₂ NaBiCl ₆	18.99	11	254.80	244	142
Cs ₂ InAsBr ₆	19.09	33	371.77	244	125
Cs ₂ RbInBr ₆	12.00	35	294.01	244	124
Cs ₂ KSbBr ₆	16.80	19	343.82	244	124
Rb ₂ LiBiBr ₆	19.83	3	321.78	220	100
Rb ₂ AlHgBr ₆	19.67	13	338.75	220	100
Cs ₂ AgBiBr ₆	19.95	35	397.73	244	124
Cs ₂ TlSbBr ₆	17.85	35	367.87	244	124
Rb ₂ AgBiBr ₆	19.54	35	399.90	220	100
Rb ₂ NaGaBr ₆	16.42	11	289.35	220	100
Rb ₂ InAsBr ₆	18.73	33	373.94	220	101
Cs ₂ KTlCl ₆	16.27	17	254.63	244	142
Cs ₂ KTlBr ₆	15.12	19	311.15	244	124
Rb ₂ InGaBr ₆	14.45	31	295.23	220	100
Cs ₂ RbBiCl ₆	14.99	17	248.96	244	142
Cs ₂ KYbCl ₆	19.74	17	306.13	244	142
Rb ₂ HgSbBr ₆	15.66	35	335.78	220	100
Rb ₂ HgBiCl ₆	16.94	17	243.32	220	118
Cs ₂ RbSbBr ₆	14.11	35	341.42	244	124
Rb ₂ NaTlCl ₆	19.52	11	260.23	220	118
K ₂ TlGaBr ₆	16.60	19	314.77	203	83
Rb ₂ HgSbCl ₆	19.90	17	279.26	220	118
Cs ₂ RbCeCl ₆	18.51	17	301.62	244	142
K ₂ NaBiBr ₆	17.12	11	318.31	203	83
Cs ₂ NaTlCl ₆	19.56	11	258.06	244	142
K ₂ RbInCl ₆	16.00	17	244.48	220	118
K ₂ InGaBr ₆	15.83	19	300.05	203	83
Cs ₂ KNdBr ₆	18.86	19	382.85	244	124
Rb ₂ TlBiBr ₆	15.44	35	334.11	220	100
K ₂ LiBiBr ₆	19.67	3	326.59	203	83
Rb ₂ TlGaBr ₆	15.18	31	309.96	220	100
Cs ₂ HgBiBr ₆	13.97	35	297.67	244	124
Cs ₂ TlInCl ₆	19.18	17	263.95	244	142
Cs ₂ RbYBr ₆	18.44	35	430.94	244	124
Cs ₂ NaTlBr ₆	18.19	11	314.58	244	124
Rb ₂ InGaCl ₆	17.35	17	238.71	220	118
Cs ₂ RbInCl ₆	14.47	17	237.49	244	142
Rb ₂ NaGaCl ₆	17.62	11	232.83	220	118
K ₂ RbAsBr ₆	18.80	19	367.03	220	101
Cs ₂ KSbCl ₆	18.48	17	287.30	244	142
K ₂ NaGaCl ₆	17.88	11	237.64	203	101
Cs ₂ HgSbCl ₆	19.96	17	277.08	244	142
Cs ₂ HgBiCl ₆	16.98	17	241.15	244	142

$K_2NaBiCl_6$	19.06	11	261.79	203	101
$K_2AlHgBr_6$	19.53	13	343.56	203	83
$K_2TlHgCl_6$	17.73	17	251.39	203	101
$Rb_2TlGaCl_6$	18.43	17	253.44	220	118
$Cs_2NaInCl_6$	18.43	11	243.34	244	142
Cs_2SBrCl_6	16.26	16	228.69	244	142
$Cs_2InAgBr_6$	19.72	35	386.26	244	124
$K_2TlSbBr_6$	19.49	19	374.86	203	83
$K_2InGaCl_6$	17.62	17	243.53	203	101
$K_2HgBiBr_6$	15.38	19	304.65	203	83
Rb_2SBrCl_6	16.25	16	230.86	220	118
Cs_2KAuBr_6	19.89	19	387.18	244	124
$Cs_2TlInBr_6$	15.50	35	320.47	244	124
$Rb_2TlSbBr_6$	17.44	35	370.05	220	100
$K_2RbInBr_6$	14.70	19	301.00	220	100
Cs_2KGaCl_6	14.53	17	227.22	244	142
$Rb_2HgAsBr_6$	17.57	33	354.40	220	101
$Rb_2NaTlBr_6$	17.81	11	316.75	220	100
$K_2RbCeBr_6$	17.77	19	365.13	220	100
$Rb_2HgBiBr_6$	13.66	35	299.84	220	100
$K_2InSbBr_6$	18.78	19	360.13	203	83
$Cs_2NaGaCl_6$	17.59	11	230.65	244	142
$K_2RbTlBr_6$	15.44	19	315.73	220	100
$Cs_2InHgBr_6$	13.63	35	286.20	244	124
$Rb_2TlInCl_6$	19.16	17	266.12	220	118
$Cs_2TlGaCl_6$	18.40	17	251.26	244	142
$Rb_2GaHgCl_6$	15.67	17	219.17	220	118
$Cs_2TlBiBr_6$	15.80	35	331.93	244	124
Cs_2KGaBr_6	13.82	19	283.74	244	124
Cs_2KCeCl_6	19.45	17	304.03	244	142
$K_2NaTlCl_6$	19.71	11	265.05	203	101
$Rb_2InAuBr_6$	19.93	35	398.68	220	100
$Cs_2TlGaBr_6$	15.46	31	307.78	244	124
$Cs_2RbTlCl_6$	15.43	17	252.22	244	142
$Cs_2InGaCl_6$	17.29	17	236.54	244	142
Cs_2KBiCl_6	15.80	17	251.37	244	142
Cs_2KPrBr_6	18.32	19	373.85	244	124
$K_2NaGaBr_6$	16.32	11	294.16	203	83
$Cs_2TlHgCl_6$	17.52	17	244.41	244	142
$K_2InHgBr_6$	15.11	19	293.19	203	83
$K_2RbSbBr_6$	17.09	19	348.41	220	100
$K_2NaInCl_6$	18.63	11	250.32	203	101
$Cs_2GaAgBr_6$	19.83	31	373.58	244	124
$Rb_2InHgCl_6$	16.45	17	231.85	220	118

Cs ₂ KAlBr ₆	18.46	13	346.79	244	124
Cs ₂ HgAsBr ₆	17.91	33	352.23	244	125
K ₂ RbGaBr ₆	14.18	19	288.32	220	100
Cs ₂ RbAsCl ₆	19.30	17	303.52	244	142
Rb ₂ TlAsBr ₆	19.42	33	388.67	220	101
Cs ₂ InHgCl ₆	16.43	17	229.68	244	142
K ₂ HgAsBr ₆	19.44	19	359.21	203	84
Na ₂ AlHgBr ₆	19.77	11	350.43	166	46
Cs ₂ RbSbCl ₆	17.57	17	284.90	244	142
Cs ₂ RbTlBr ₆	12.65	35	308.74	244	124
Cs ₂ KInBr ₆	14.37	19	296.42	244	124
K ₂ RbSbCl ₆	19.21	17	291.89	220	118
K ₂ NaInBr ₆	16.85	11	306.84	203	83
K ₂ TlHgBr ₆	15.86	19	307.91	203	83
Cs ₂ KCeBr ₆	17.52	19	360.55	244	124
Cs ₂ RbGaCl ₆	13.74	17	224.81	244	142
Cs ₂ InGaBr ₆	14.70	31	293.06	244	124
Cs ₂ TlAsBr ₆	19.81	33	386.49	244	125
Rb ₂ NaInCl ₆	18.42	11	245.51	220	118
Cs ₂ InBiCl ₆	18.61	17	260.69	244	142
Cs ₂ RbGaBr ₆	11.89	31	281.33	244	124
Cs ₂ GaHgCl ₆	15.61	17	217.00	244	142
Rb ₂ InAgBr ₆	19.37	35	388.44	220	100
Cs ₂ KBiBr ₆	14.73	19	307.89	244	124
K ₂ NaTlBr ₆	17.64	11	321.57	203	83
Cs ₂ AgBiBr ₆	19.95	35	397.73	244	124
Rb ₂ TlHgBr ₆	14.08	35	303.10	220	100
K ₂ HgBiCl ₆	17.12	17	248.13	203	101
Na ₂ LiBiBr ₆	19.45	3	333.46	166	46
Cs ₂ InSbBr ₆	17.15	35	353.15	244	124
K ₂ RbAlBr ₆	18.87	13	351.37	220	100
Rb ₂ NaBiCl ₆	18.91	11	256.97	220	118
Rb ₂ GaHgBr ₆	13.28	31	275.69	220	100
K ₂ RbBiBr ₆	15.01	19	312.47	220	100
Cs ₂ IBrCl ₆	15.38	17	228.54	244	142
Rb ₂ InSbBr ₆	16.77	35	355.32	220	100
Cs ₂ RbAlBr ₆	17.60	13	344.39	244	124
Cs ₂ HgAuBr ₆	19.12	35	376.96	244	124
Rb ₂ HgAuBr ₆	18.77	35	379.13	220	100
Cs ₂ RbAlCl ₆	19.14	13	287.87	244	142
Cs ₂ RbPrCl ₆	19.51	17	314.92	244	142
K ₂ InHgCl ₆	16.69	17	236.67	203	101
Rb ₂ TlHgCl ₆	17.52	17	246.58	220	118