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Electronic Supporting Information for

Hierarchical computational screening of layered lead-free metal halide perovskites for optoelectronic applications

Qiuqi Liu,[a] Dan Cao,[a,] Xueyin Liu,[b] Xiangyu Zhou,[b] and Xiaoshuang Chen,[c] Haibo Shu[b,*]*

[a]College of Science and [b]College of Optical and Electronic Technology, China Jiliang University, 310018 Hangzhou, China

[c]National Laboratory for Infrared Physics, Shanghai Institute of Technical Physics, Chinese Academy of Science, 200083 Shanghai, China

[*]Corresponding author. Haibo Shu, E-mail: shuhaibo@cjlu.edu.cn, Phone: 86-0571-86875622; Dan Cao, E-mail: caodan@cjlu.edu.cn, Phone: 86-0571-86835756.

S1. Lattice and energetic parameters of cubic ABX_3 perovskites

Table S1. Lattice constants *a*, tolerance factors *t*, and formation energies E_f of cubic MHPs with the general formula of ABX_3.

ABX_3	*a* (Å)	*t*	E_f (eV)
$LiGeF_3$	4.3794	0.6613	1.9929
$LiSnF_3$	4.6747	0.6052	2.3271
$LiPbF_3$	4.4243	0.5414	3.6130
$LiGeCl_3$	5.2059	0.6709	2.0597
$LiSnCl_3$	5.5472	0.6219	1.6330
$LiPbCl_3$	5.6717	0.5661	1.7700
$LiGeBr_3$	5.4721	0.6728	1.3156
$LiSnBr_3$	5.8139	0.6261	1.4933
$LiPbBr_3$	5.9440	0.5724	1.5961
$LiGeI_3$	5.8798	0.6753	1.3960
$LiSnI_3$	6.1984	0.6316	1.4144
$LiPbI_3$	6.3137	0.5808	1.6755
$NaGeF_3$	4.3956	0.7815	0.1506
$NaSnF_3$	4.6837	0.7133	0.3471
$NaPbF_3$	4.8114	0.6381	0.1446
$NaGeCl_3$	5.2210	0.7684	-0.3091
$NaSnCl_3$	5.5544	0.7123	-0.1764
$NaPbCl_3$	5.6645	0.6484	-0.5067
$NaGeBr_3$	5.4908	0.7652	-0.3554
$NaSnBr_3$	5.8229	0.7120	-0.2577
$NaPbBr_3$	5.9435	0.6510	-0.2001
$NaGeI_3$	5.8923	0.7609	-0.2073
$NaSnI_3$	6.2138	0.7117	0.0472
$NaPbI_3$	6.3352	0.6545	0.0472
$KGeF_3$	4.4221	0.9101	0.0212
$KSnF_3$	4.7238	0.8306	0.2143
$KPbF_3$	4.8388	0.7430	0.3588
$KGeCl_3$	5.2712	0.8741	0.6821
$KSnCl_3$	5.5800	0.8103	0.1538
$KPbCl_3$	5.6830	0.7376	0.2713
$KGeBr_3$	5.5426	0.8654	-0.0543
$KSnBr_3$	5.8486	0.8053	-0.0239
$KPbBr_3$	5.9513	0.7363	0.1685
$KGeI_3$	5.9313	0.8540	0.2555
$KSnI_3$	6.2342	0.7986	0.1882

$KPbI_3$	6.3534	0.7345	0.4065
$RbGeF_3$	4.4893	0.9608	-0.1808
$RbSnF_3$	4.7509	0.8769	-0.0631
$RbPbF_3$	4.8014	0.7844	0.0730
$RbGeCl_3$	5.2916	0.9159	0.3638
$RbSnCl_3$	5.5903	0.8490	-0.0891
$RbPbCl_3$	5.7076	0.7729	0.0158
$RbGeBr_3$	5.5693	0.9050	-0.2134
$RbSnBr_3$	5.8711	0.8421	-0.2252
$RbPbBr_3$	5.9797	0.7700	-0.1408
$RbGeI_3$	5.9602	0.8906	0.1106
$RbSnI_3$	6.2514	0.8330	0.0109
$RbPbI_3$	6.3681	0.7660	0.2202
$CsGeF_3$	4.5573	1.0319	-0.2125
$CsSnF_3$	4.7947	0.9418	-0.2397
$CsPbF_3$	4.8991	0.8425	-0.1861
$CsGeCl_3$	5.3402	0.9744	0.2549
$CsSnCl_3$	5.6150	0.9032	-0.3327
$CsPbCl_3$	5.7320	0.8222	-0.2268
$CsGeBr_3$	5.6049	0.9604	-0.3292
$CsSnBr_3$	5.8832	0.8937	-0.2646
$CsPbBr_3$	6.0042	0.8171	-0.3398
$CsGeI_3$	5.9958	0.9420	-0.0091
$CsSnI_3$	6.2760	0.8810	-0.1564
$CsPbI_3$	6.3884	0.8102	0.0396

S2. The SOC effect on band structures of Pb-free ABX_3 perovskites

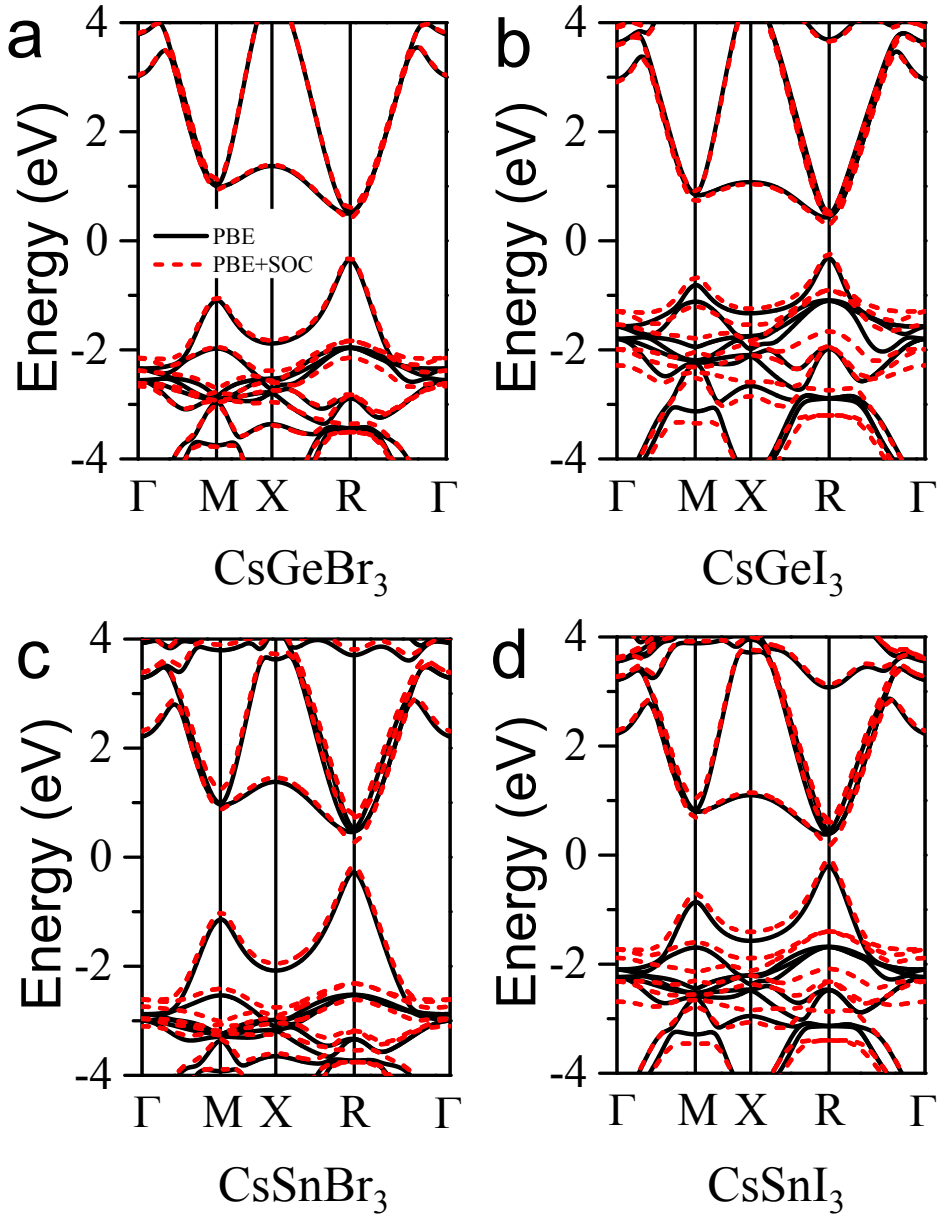

Fig. S1 Band structures of (a) $CsGeBr_3$, (b) $CsGeI_3$, (c) $CsSnBr_3$, and (d) $CsSnI_3$ calculated by the PBE functional. The dash lines and solid lines denote the band structures calculated with and without the SOC effect, respectively.

S3. The effect of vdW interaction on lattice parameters of layered perovskites

For the layered Pb-free perovskites, the interlayer vdW interactions play an important role in their geometrics and stabilities. In order to understand this issue, we used D-J phase $PRSnBr_4$ (D-J-1) as an example to compare with its lattice parameters with respect to different vdW corrections, as listed in Table S2. It is a well-known fact that the PBE functional usually induces the overestimation of lattice constants and interlayer distance. In contrast, PBE-D3 functional makes relatively smaller lattice constants and interlayer distance in D-J-1 than the PBE functional, thus the calculated results from PBE-D3 more approach the experimental values. For the PBE-sol functional, its result is largely similar to that of PBE functional. Based on above reasons, the PBE functional with the D3 correction was used in this work.

Table S2 Lattice constants (a, b, c), interlayer distances (D), bond lengths (l), and bond angles (θ) of D-J phase $PRSnBr_4$ obtained with different vdW corrections.

					l **(Å)**			***θ*** **(°)**		
D-J-1	***a*** **(Å)**	***b*** **(Å)**	***c*** **(Å)**	***D*** **(Å)**	$l_{Sn\text{-}Br}$ (x)	$l_{Sn\text{-}Br}$ (y)	$l_{Sn\text{-}Br}$ (z)	$\theta_{Br\text{-}Sn\text{-}Br}$ (x)	$\theta_{Br\text{-}Sn\text{-}Br}$ (y)	$\theta_{Br\text{-}Sn\text{-}Br}$ (z)
PBE	5.89	5.86	16.61	10.65	2.78	2.98	2.99	162.2	159.4	169.7
PBE-D2	5.69	5.67	16.05	10.12	2.78	2.87	2.99	165.3	163.6	171.8
PBE-D3	5.76	5.74	16.24	10.30	2.79	2.90	2.99	165.1	162.3	171.6
PBE-sol	5.86	5.84	16.52	10.70	2.81	2.94	2.95	162.3	166.2	168.0

S4. The convergence of energy and optical absorption spectra in 2D Pb-free perovskites with respect to the k-point mesh

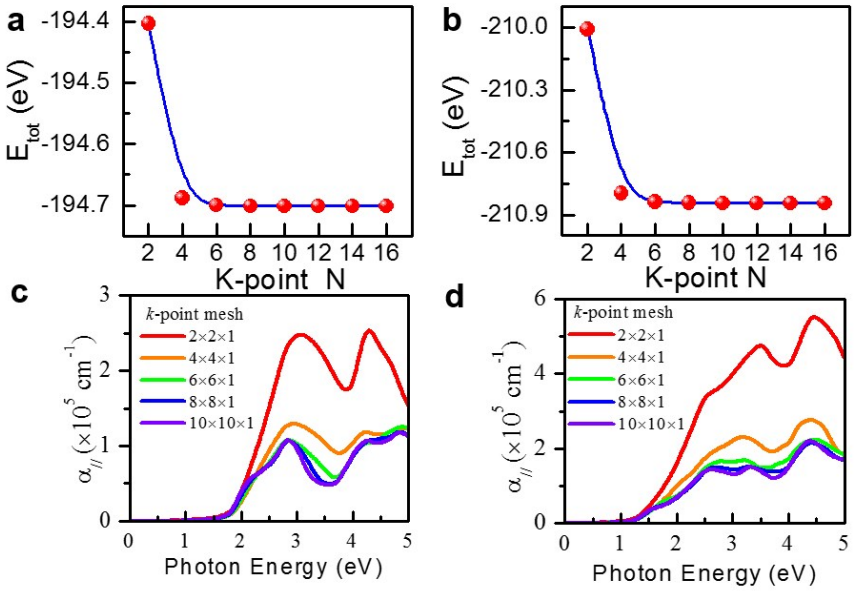

Fig. S2 Total energies (E_{tot}) of $BA_2Cs_{n-1}Sn_nBr_{3n+1}$ with (a) n = 1 and (b) n = 2 as a function of k-point value N (i.e., k-point mesh is N × N × 1). The convergence of optical absorption spectra in $BA_2Cs_{n-1}Sn_nBr_{3n+1}$ with (c) n = 1 and (d) n = 2 with the respect to the k-point mesh.

S5. Band structures of cubic Pb-free ABX_3 perovskites

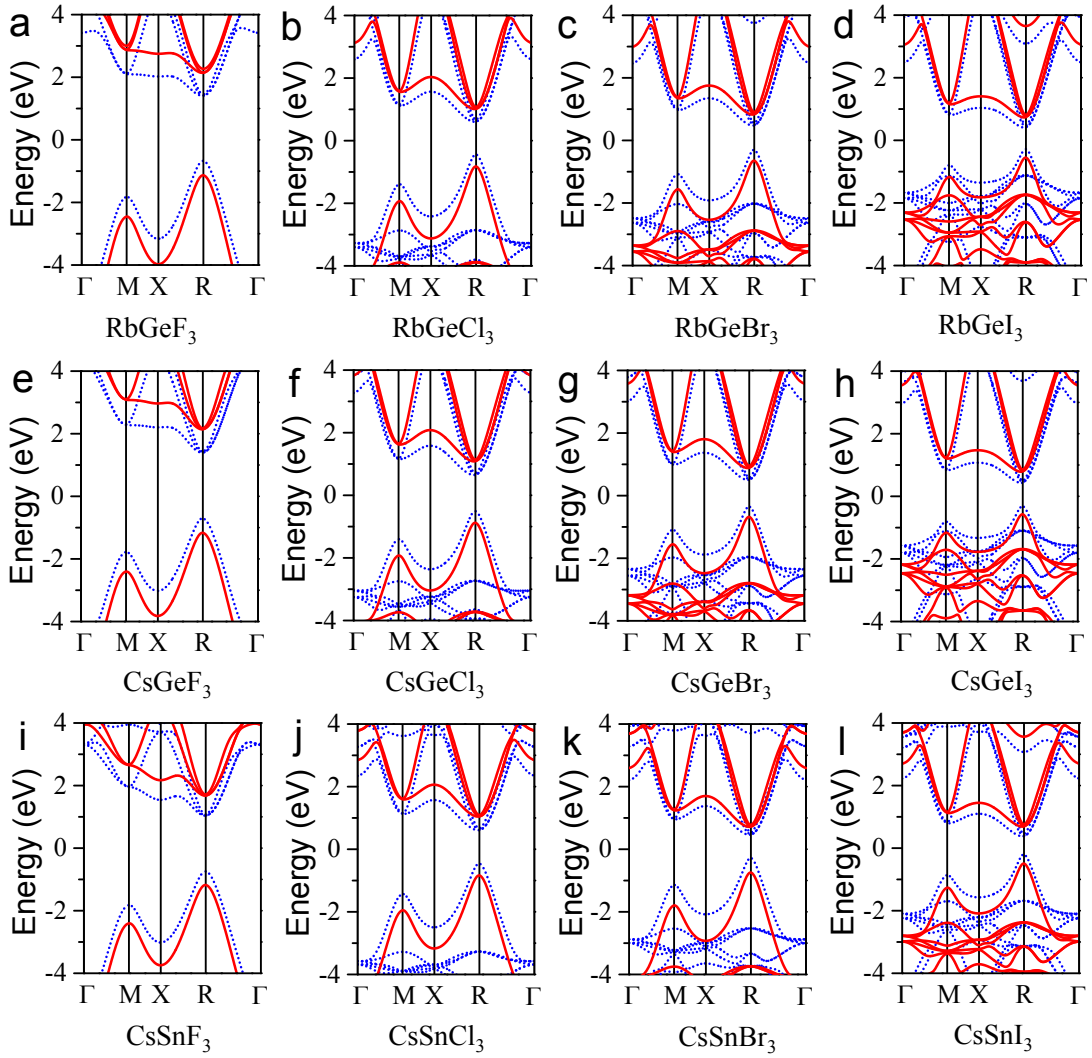

Fig. S3 Band structures of cubic Pb-free ABX_3 perovskites. (a) $RbGeF_3$, (a) $RbGeCl_3$, (c) $RbGeBr_3$, (d) $RbGeI_3$, (e) $CsGeF_3$, (f) $CsGeCl_3$, (g) $CsGeBr_3$, (h) $CsGeI_3$, (i) $CsSnF_3$, (j) $CsSnCl_3$, (k) $CsSnBr_3$, and (l) $CsSnI_3$. The band structures calculated by the HSE06 and PBE functional are indicated by solid and dash curves, respectively.

S6. Density of states of $CsSnX_3$ (X = F, Cl, Br, and I)

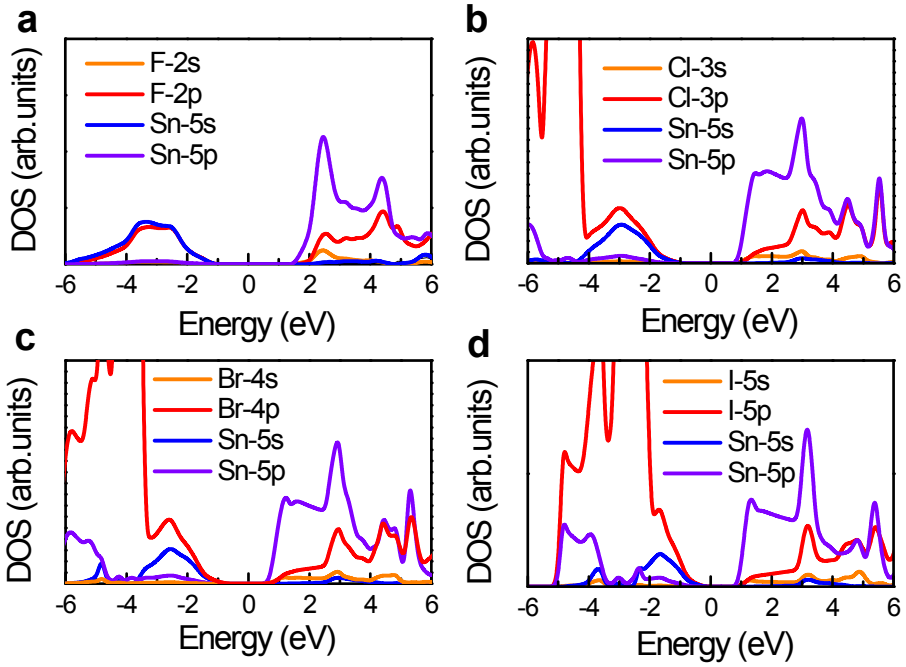

Fig. S4 Partial density of states (PDOS) of Sn-5s, 5p and halogen X-s, p orbitals in (a) $CsSnF_3$, (b) $CsSnCl_3$, (c) $CsSnBr_3$, and (d) $CsSnI_3$. The energy zero point corresponds to the position of Fermi level.

S7. Lattice parameters and adsorption energies of $A'_2Cs_{n-1}Sn_nBr_{3n+1}$ nanosheets

Table S3 Total atomic numbers N_{tot}, lattice constants a and b, average bond lengths l, and bond angles θ of 2D $A'_2Cs_{n-1}Sn_nBr_{3n+1}$ (n = 1, 2) nanosheets with different organic cations A′. The details about the optimized structures of these 2D perovskites used in DFT calculations (i.e, POSCAR files) are attached in the section of S10.

Organic cations	n	N_{tot}	a (Å)	b (Å)	Bond lengths l (Å)			Bond angles θ (°)		
					l_{Sn-Br} (x)	l_{Sn-Br} (y)	l_{Sn-Br} (z)	$\theta_{Br-Sn-Br}$ (x)	$\theta_{Br-Sn-Br}$ (y)	$\theta_{Br-Sn-Br}$ (z)
BA	1	39	5.96	5.93	3.27	2.98	3.07	161.8	160.9	169.9
	2	44	5.92	5.89	2.95	2.96	2.98	170.3	167.2	168.3
PEA	1	47	5.94	5.92	2.76	2.99	2.98	161.7	159.7	169.7
	2	52	5.94	5.93	2.90	3.02	2.96	168.8	166.2	171.3
EA	1	27	5.90	5.86	2.90	3.02	3.02	166.9	171.8	165.4
	2	32	5.93	5.88	2.80	2.97	2.99	167.1	165.0	169.5
DMA	1	27	6.03	6.00	3.29	3.14	3.05	177.9	178.0	175.8
	2	32	6.03	5.99	3.29	3.15	2.53	170.2	177.6	177.8
MA	1	21	5.85	5.85	3.13	3.13	3.02	155.1	155.1	157.9
	2	26	5.94	5.98	2.95	3.02	3.15	174.0	176.2	176.0
PMA	1	41	5.97	5.94	2.84	3.05	3.02	167.2	173.9	173.6
	2	46	5.97	5.94	2.99	3.06	2.99	176.4	173.9	176.9
GA	1	25	6.35	6.34	3.60	3.58	3.00	175.8	170.8	178.6
	2	30	6.26	6.25	2.77	3.49	2.99	173.1	174.0	172.6

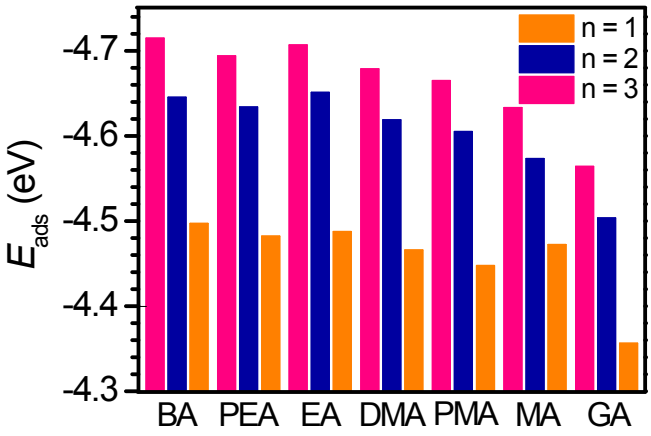

Fig. S5 Adsorption energies (E_{ads}) of $A'_2Cs_{n-1}Sn_nBr_{3n+1}$ (n = 1, 2, 3) nanosheets with different organic cations.

S8. Phonon dispersions of $BA_2Cs_{n-1}Sn_nBr_{3n+1}$ (n=1, 2)

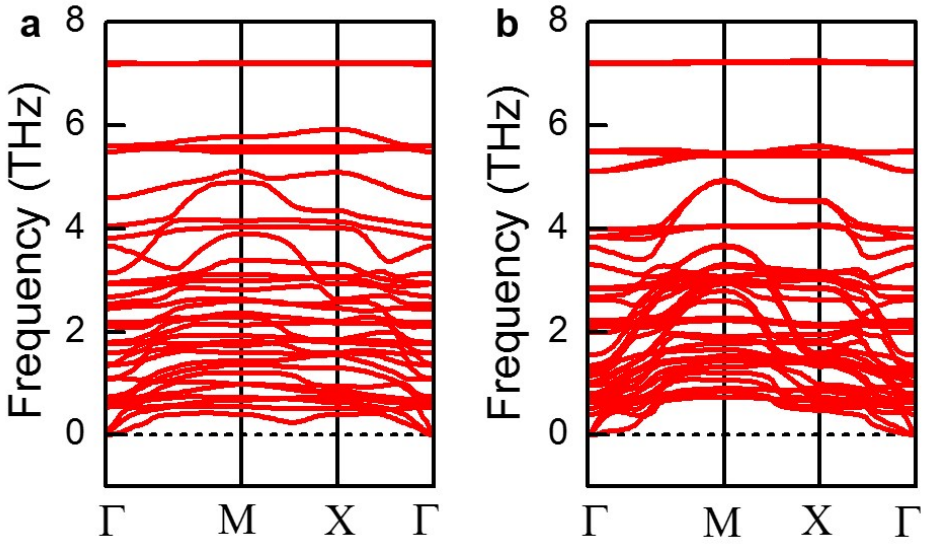

Fig. S6 Phonon dispersions of (a) BA_2SnBr_4 and (b) $BA_2CsSn_2Br_7$. The position of dash lines corresponds to the zero point of phonon frequency.

S9. Optimized lattice parameters of 2D layered Pb-free MHPs

Table S4 Total atomic numbers N_{tot}, lattice constants a, b, and c, interlayer distance D, average bond lengths l, and bond angles θ of R-P and D-J phase layered perovskites. Here T and B denote the top and bottom layer, respectively. The details about the optimized structures of these layered perovskites used in DFT calculations (i.e, POSCAR files) are attached in the section of S13.

Phase	N_{tot}	a (Å)	b (Å)	c (Å)	D (Å)	Layer	Bond lengths l (Å)			Bond angles θ (°)		
							l_{Sn-Br} (x)	l_{Sn-Br} (y)	l_{Sn-Br} (z)	$\theta_{Br-Sn-Br}$ (x)	$\theta_{Br-Sn-Br}$ (y)	$\theta_{Br-Sn-Br}$ (z)
R-P-1	156	11.55	5.76	34.54	11.31	T	2.82	2.94	3.04	166.3	162.9	173.9
						B	2.81	2.93	3.03	167.5	163.8	173.1
R-P-2	176	11.57	5.78	45.93	11.19	T	2.90	2.90	2.97	171.4	170.4	169.4
						B	2.90	2.90	2.97	171.4	170.3	169.2
D-J-1	37	5.76	5.74	16.24	10.30	T	2.79	2.90	2.99	165.1	162.3	171.6
						B	2.79	2.90	2.99	165.1	162.3	171.6
D-J-2	42	5.83	5.82	21.68	9.99	T	2.92	2.92	2.96	171.5	169.7	169.5
						B	2.92	2.92	2.96	171.5	169.7	169.5
D-J-3	47	5.83	5.82	27.41	9.87	T	2.92	2.92	2.95	173.4	173.1	172.4
						B	2.92	2.92	2.95	173.4	173.1	172.4

S10. AIMD simulation results of 2D layered Pb-free MHPs

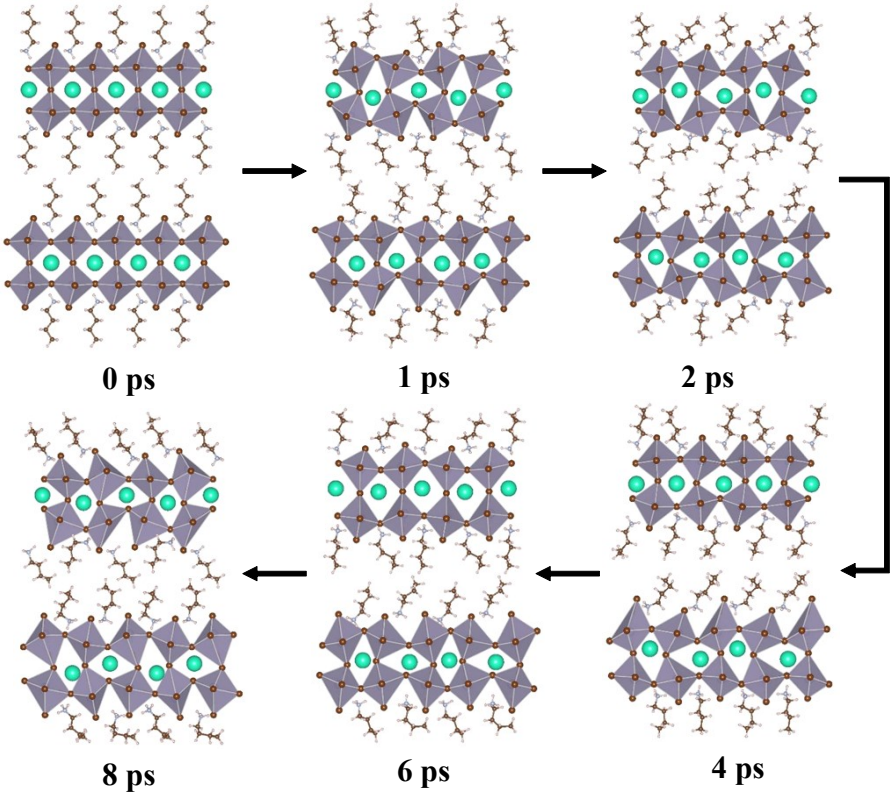

Fig. S7 Snapshots of AIMD trajectories of R-P phase $BA_2CsSn_2Br_7$ (R-P-2) within the simulation time of 8 ps.

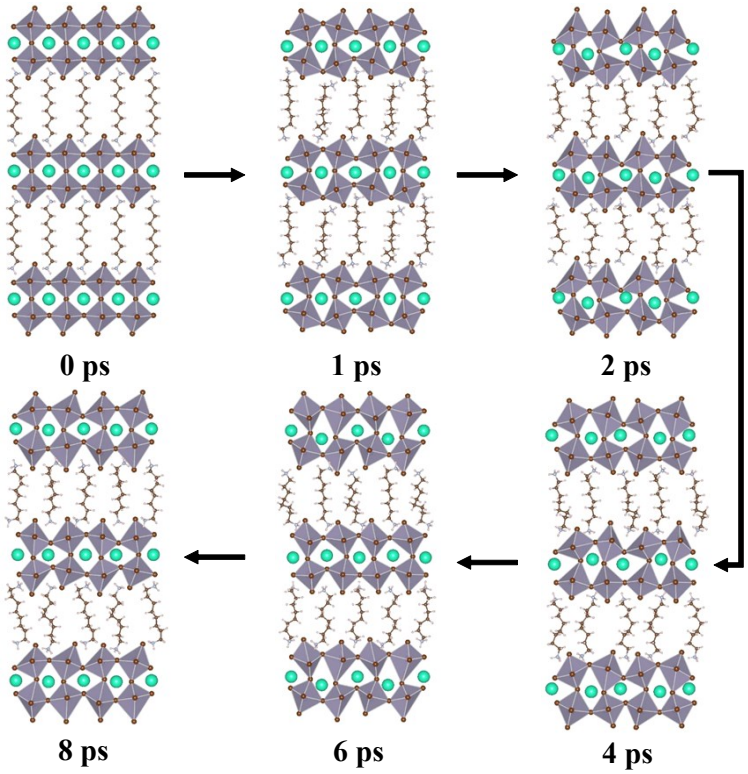

Fig. S8 Snapshots of AIMD trajectories of D-J phase $PRCsSn_2Br_7$ (D-J-2) within the simulation time of 8 ps.

Table S5 Bond lengths (l) and bond angles (θ) of R-P phase $BA_2CsSn_2Br_7$ (R-P-2) and D-J phase $BA_2CsSn_2Br_7$ (D-J-2) with the simulation time of AIMD at 0 ps and 8 ps.

Phase	Time	Layer	Bond lengths l (Å)			Bond angles θ (°)		
			$l_{\text{Sn-Br}}(x)$	$l_{\text{Sn-Br}}(y)$	$l_{\text{Sn-Br}}(z)$	$\theta_{\text{Br-Sn-Br}}$ (x)	$\theta_{\text{Br-Sn-Br}}$ (y)	$\theta_{\text{Br-Sn-Br}}$ (z)
R-P-2	0 ps	Top	2.90	2.90	2.97	171.4	170.4	169.4
		Bottom	2.90	2.90	2.97	171.4	170.3	169.2
	8 ps	Top	3.46	3.00	2.78	145.2	169.8	137.6
		Bottom	3.09	2.90	3.85	144.0	172.2	164.3
D-J-2	0 ps	Top	2.92	2.92	2.96	171.5	169.7	169.5
		Bottom	2.92	2.92	2.96	171.5	169.7	169.5
	8 ps	Top	3.21	2.73	2.90	158.5	172.3	164.2
		Bottom	3.21	2.73	2.90	158.5	172.3	164.2

S11. AIMD simulation results of $CsSnBr_3$ thin film and layered Pb-free MHPs in the moisture environment

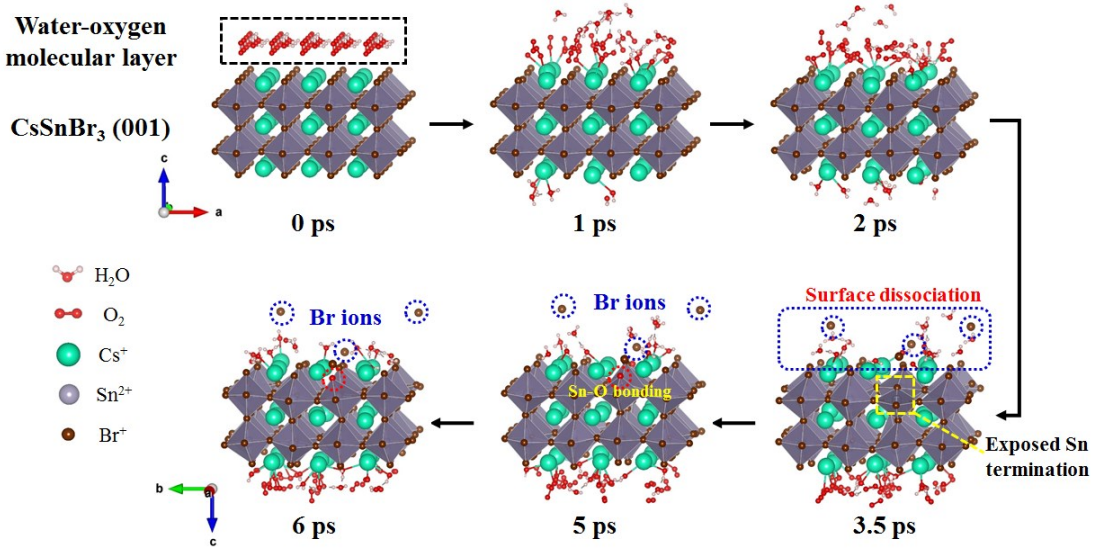

Fig. S9 Snapshots of AIMD trajectories of $CsSnBr_3$(001) thin film with a water-oxygen molecular layer following 6 ps AIMD simulation at 300 K.

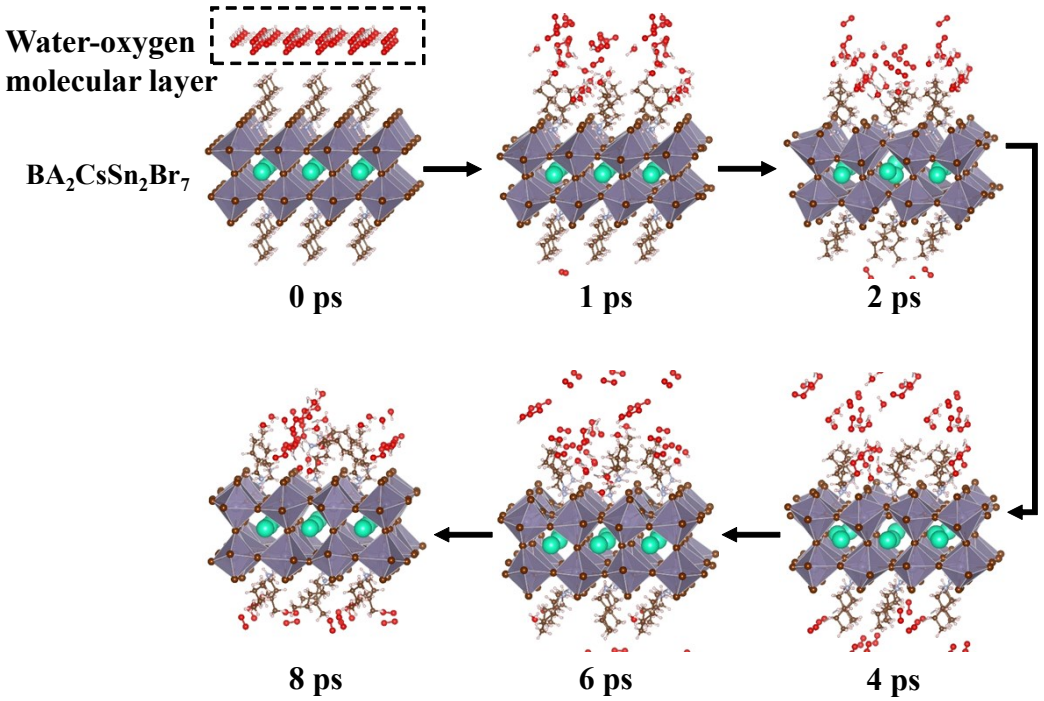

Fig. S10 Snapshots of AIMD trajectories of $(BA)_2CsSn_2Br_7$ with a water-oxygen molecular layer following 8 ps AIMD simulation at 300 K.

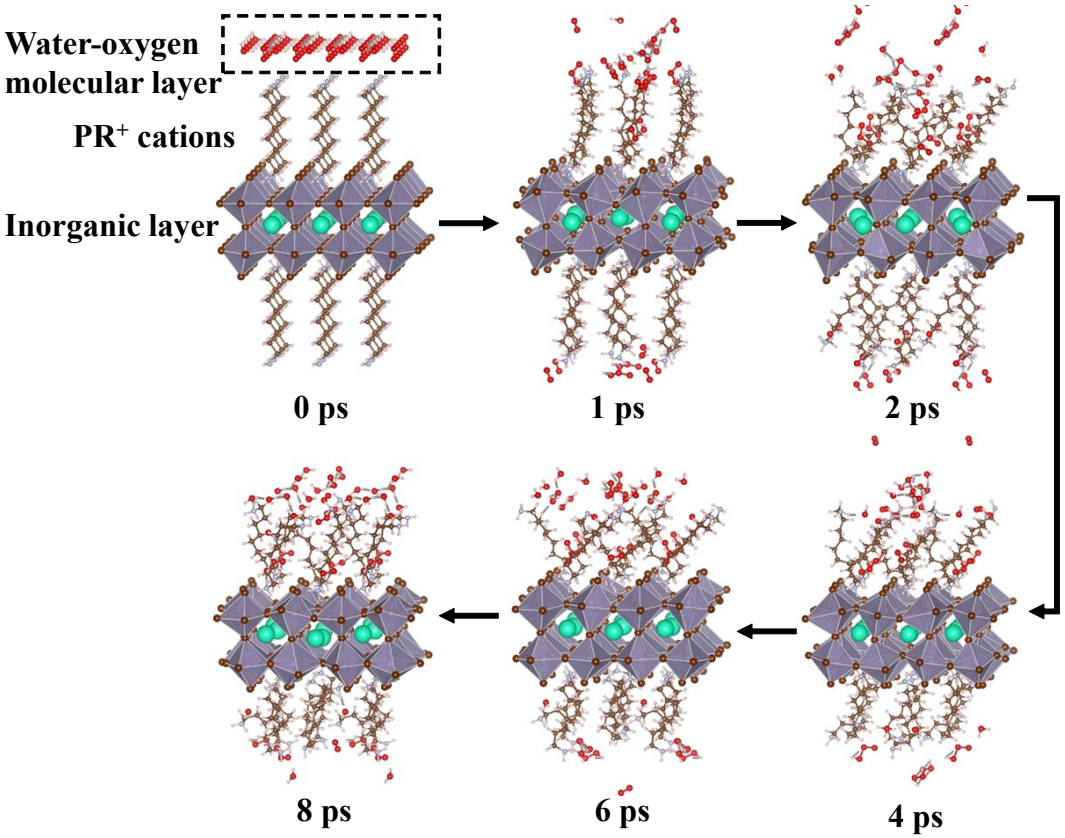

Fig. S11 Snapshots of AIMD trajectories of $PRCsSn_2Br_7$ with a water-oxygen molecular layer following 8 ps AIMD simulation at 300 K.

S12. The comparison of PCE models

The maximum PCE is a key parameter to evaluate the potential of semiconductor materials as the absorber of solar cells. In previous literatures[1-3], the maximum PCE (η) was estimated by widely using the formula proposed by Scharber et al.[4]

$$\eta=\frac{FF\cdot V_{oc}\cdot J_{sc}}{P_{solar}}=\frac{FF\times(E_g-\Delta E_c-0.3)\int_{E_g}^{\infty}\frac{S(E)}{E}dE}{\int_0^{\infty}S(E)dE} \quad (1)$$

where FF is the fill factor that is usually set to 0.65, $E_g - \Delta E_C - 0.3$ is an estimate of the maximum open circuit voltage V_{oc}, $S(E)$ is the AM1.5 solar energy flux (stated in W/m^2 eV) at the photon energy E, and E_g is the band gap of a given semiconductor absorber. However, this model ignore the influence of absorption coefficient and thickness of absorber layer on the PCE. In other words, the maximum PCE is mainly related to the band gap of the semiconductor absorber irrespective of its absorption coefficient, material thickness, and light-irradiation direction. Such a strategy induces an overestimation of PCE value. As listed in Table S6, the calculated PCE of 2D BA_2SnBr_4 and $BA_2CsSn_2Br_7$ is 10.66% and 19.23% for the light irradiation along their out-of-plane direction, respectively. Obviously, the predicted PCE values are not reasonable because of photons cannot be effectively absorbed by ultrathin nanosheets. On the other hand, spectroscopic limited maximum efficiency (SLME) method has also been developed to predict the maximum PCE as follows[5],

$$\eta=\frac{eV\int_0^{\infty}a(E)I_{sun}(E)dE-\frac{eV\pi}{f_r}(1-e^{-eV/kT})\int_0^{\infty}a(E)I_{bb}(E,T)dE}{eV\int_0^{\infty}I_{sun}(E)dE} \quad (2)$$

where I_{sun} is the photon flux, e is the elementary charge, I_{bb} is the black-body spectrum, k is the Boltzmann constant, V is the open circuit voltage. $a(E)$ is the photon absorption factor and it can be written as $a(E)=1-e^{-2\alpha(E)L}$, where $\alpha(E)$ is the calculated absorption coefficient and L is the thickness of the structure. f_r is the fraction of radiative recombination current, written as $f_r=e^{-(E_g^{da}-E_g)/kT}$, where E_g^{da} is the electric-dipole-allowed direct optical transition and E_g is the band gap. The

impact of optical absorption on the PCE is considered in the SLME model. However, SLME model does not depend on the magnitude of fill factor *FF*. Hence, we develop an improved PCE model by introducing the absorption factor *a(E)* into Scharber's formula as follows,

$$\eta=\frac{FF\cdot V_{oc}\cdot J_{sc}}{P_{solar}}=\frac{FF\times(E_g-E_{loss})\int_{E_g}^{\infty}a(E)\frac{S(E)}{E}dE}{\int_{0}^{\infty}S(E)dE} \tag{3}$$

In this model, the PCE of semiconductor absorbers can be related to the absorption coefficient and material thickness (*L*). As shown in Fig. S12, we present the PCE values of R-P and D-J phase layered MHPs as a function of material thickness *L*. It can be found that the PCE values of these layered structures increase with their thicknesses and have few changes when *L* is beyond ~500 nm. For obtaining the maximum PCE, thus *L* is set 500 nm in this work.

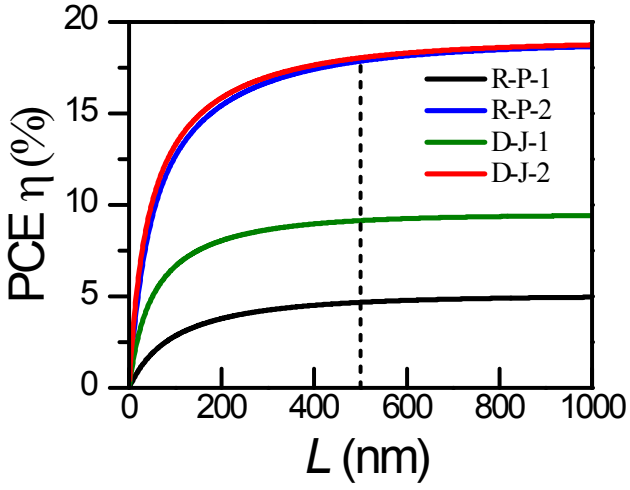

Fig. S12 PCE (η) of R-P and D-J phase layered perovskites as a function of material thickness (*L*).

In order to examine the reasonability of three models for the prediction of PCE, we use the experimental results of $CsSnBr_3$-based solar cell reported by Gupta et al.[6] as input parameters, including band gap (1.75 eV), fill factor *FF* (0.56), open voltage V_{OC} (0.4 V), thickness of $CsSnBr_3$ layer (300 nm), and absorption coefficients. The obtained PCE value is 4.72% and 16.60% for using Scharber's model and SLME model, respectively. In contrast, the improved model leads to the PCE value of 2.25% that is in good agreement with the experimental value (2.1%). In addition, we have

made a comparison between the Scharber's model and our improved model to predict the maximum PCE for various Sn-based perovskites (Table S6). It can be found that $\eta_{//}$ of these perovskites calculated by the improved model is slightly lower than that obtained by the Scharber's model. However, two models lead to a large difference of $\eta_{\perp}$ for these perovskites. For example, $\eta_{\perp}$ of 2D BA_2SnBr_4 nanosheet is 10.83% and 0.02% for the use of Scharber's model and our improved model, respectively. It is easy to understand that the atomically thin BA_2SnBr_4 nanosheet is impossible to show a larger $\eta_{\perp}$ due to the weak utilization of photons. Therefore, the improved model can provide a more reasonable prediction of PCE values.

Table S6 The maximum PCE η (%) of various Sn-based perovksites calculated by using Scharber formula and improved model. $\eta_{//}$ and $\eta_{\perp}$ denote the PCE obtained by considering light irradiation along the in-plane and out-of-plane direction of the perovskite materials, respectively.

PCE model	η	$CsSnBr_3$	BA_2SnBr_4	$BA_2CsSn_2Br_7$	R-P-1	R-P-2	D-J-1	D-J-2
Scharber	$\eta_{//}$	23.42	10.83	19.53	5.10	19.15	9.60	19.22
	$\eta_{\perp}$	23.42	10.83	19.53	5.10	19.15	9.60	19.22
This work	$\eta_{//}$	21.34	9.94	18.10	4.75	16.02	9.28	18.32
	$\eta_{\perp}$	21.34	0.02	0.18	2.44	11.27	4.27	12.95

S13. The structural files (POSCAR) of 2D and layered Pb-free MHPs

(1) BA_2SnBr_4

2D-1-BA2SnBr4

1.00000000000000

5.9628011384114128 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.9257368249900804 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

H C N Br Sn

24 8 2 4 1

Selective dynamics

Direct

0.1732925731284114 0.8539432665779921 0.3673673817423423 T T T

0.1743317921345949 0.1530076077920910 0.3688795819140794 T T T

0.8352125113785547 0.8468263707316137 0.4106972316781252 T T T

0.8350983448994667 0.1466528543217834 0.4120861352354724 T T T

0.2074850043640348 0.8488174959983429 0.4391184059178077 T T T

0.0190270305058805 0.9852464030159784 0.4663839481161097 T T T

0.7900545880968091 0.1589320555803624 0.3390129722424258 T T T

0.7889096431072674 0.8615119578671747 0.3374780110848105 T T T

0.1259915917229282 0.8670348196659706 0.2934503522143038 T T T

0.1273662351728855 0.1664450478844444 0.2950212389705544 T T T

0.8985016113251066 0.0215533852312792 0.2737360505801519 T T T

0.2063511112205299 0.1354062417676035 0.4406343306114562 T T T

0.8483841682681982 0.8517517080627656 0.6616760791485029 T T T

0.8487299128823157 0.1505702450750475 0.6593741196159967 T T T

0.1480971904912226 0.8364472250439740 0.6109535862451210 T T T

0.1499670005213947 0.1374109574039623 0.6088737286879896 T T T

0.7550854191938873 0.8413998811369234 0.5923525038793670 T T T

0.9125669614188736 0.9685074918375453 0.5598549389337490 T T T

0.2518532188157093 0.1550273870972803 0.6807091697114575 T T T

0.2512784949358831 0.8576293741302730 0.6830943174195445 T T T

0.9478362458254765 0.8714449284148288 0.7337268984897632 T T T

0.9483539993496349 0.1706286357625263 0.7313134821214452 T T T

0.1890161018253783 0.0250277392865297 0.7482292913739192 T T T

0.7603438086463301 0.1300765292148834 0.5894185654333074 T T T

0.0640565300330296 0.0035718750221998 0.3697809101375478 T T T

0.9418391380239073 0.9973528596003793 0.4079685590311097 T T T

0.8999671795008328 0.0101757461511078 0.3361257749222654 T T T

0.0192006841738957 0.0166490690108810 0.2974578239662029 T T T

0.9562745045705330 -0.0000419717352097 0.6564381766589794 T T T

0.0469186851695830 0.9889738948002863 0.6157750275773630 T T T

0.1436333376221274 0.0077839045990922 0.6863237995190234 T T T

0.0526041368153951 0.0193414279482766 0.7271322593606417 T T T

0.1046075352603063 0.9918905945733669 0.4406891351993513 T T T
0.8573989779187630 0.9829550813169349 0.5877064635476312 T T T
0.5963391511383181 0.0112086609904195 0.5014316013312148 T T T
0.4090260125281077 0.4989273544370491 0.4267816797540856 T T T
0.5720693652381881 0.4869521266691168 0.5969393018861355 T T T
0.0710935065632892 0.5557761722965407 0.5212863347153728 T T T
0.5280306962129461 0.5146805954183666 0.5096938310253064 T T T

(2) $BA_2CsSn_2Br_7$

2D-2-BA2CsSn2Br7-

1.00000000000000

5.9203875939241879 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.8902111833660973 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

H C N Br Sn Cs

24 8 2 7 2 1

Selective dynamics

Direct

0.1634357015735449 0.8518856121399100 0.2806443467714588 T T T
0.1641167094570533 0.1527780153523919 0.2810368720377850 T T T
0.8283359603437713 0.8496478684572104 0.3251461019086669 T T T
0.8278504029549371 0.1519332790087700 0.3253819251385299 T T T
0.2074571048770907 0.8565673644881522 0.3517804814923342 T T T
0.0254315827153901 0.9998456696885645 0.3795706017852085 T T T
0.7745752223324291 0.1542277859654440 0.2520796927355656 T T T
0.7740179604200619 0.8548639711314741 0.2516382947438048 T T T
0.1115953172317575 0.8557069124326975 0.2071091388422647 T T T
0.1117693879397978 0.1570640694281848 0.2075281847529569 T T T
0.8809778437886165 0.0075133775733986 0.1870848162974977 T T T
0.2072198210550181 0.1446226428370072 0.3519471639266400 T T T
0.8586842131225355 0.8522816707032040 0.7306928006706447 T T T
0.8575932335715667 0.1531923463534504 0.7302907341234509 T T T
0.2002472469238344 0.8507409074644517 0.6875760712659038 T T T
0.2002524134760061 0.1527275841757380 0.6873412216798869 T T T
0.8258869748210179 0.8570707864963927 0.6590928818357807 T T T
0.0144960580032570 0.0006541198191632 0.6323524710491285 T T T
0.2432387136651948 0.1553982959287353 0.7606860853848078 T T T
0.2445505465752646 0.8560670097888705 0.7610898043219476 T T T
0.9015033208455937 0.8557703686716984 0.8043985940777219 T T T
0.9007978866317612 0.1571392518210106 0.8040669813376684 T T T
0.1293466456984029 0.0077935133733043 0.8252658027789906 T T T
0.8256761649323557 0.1447521264749756 0.6589518971842605 T T T
0.0532905253974109 0.0024844958680349 0.2828029865135733 T T T
0.9346668576750456 0.0010756126867342 0.3214024987911661 T T T

0.8853776748107879	0.0044585002794208	0.2495283819478707	T	T	T
0.0035120678681259	0.0062800208023770	0.2106720784217991	T	T	T
0.9688181385020972	0.0030617455047146	0.7289494782437115	T	T	T
0.0929323557034714	0.0018337276589098	0.6908608195090701	T	T	T
0.1325109883667932	0.0053337864611966	0.7628250130523729	T	T	T
0.0096868114459043	0.0065979211999518	0.8012598070558016	T	T	T
0.1044259728970123	0.0005261416389096	0.3532946343371933	T	T	T
0.9288914497639520	0.0010149423528825	0.6581076847524796	T	T	T
0.5560688761489516	0.0016895944103046	0.4196352341902526	T	T	T
0.4432482427120522	0.0008666850162525	0.5950226128521299	T	T	T
0.4167999151343426	0.5017376743144568	0.3369805132433510	T	T	T
0.4998337408061175	0.5010538747091948	0.5062240535353850	T	T	T
0.6114137029949668	0.5021306569577325	0.6749405692755232	T	T	T
0.0276115778853023	0.5024767720428320	0.4266376249733225	T	T	T
0.9783146902166964	0.5010031274455018	0.5834362216318438	T	T	T
0.5082210318513247	0.5017594968580249	0.4208631086124113	T	T	T
0.5035304624983991	0.5009658750072660	0.5920354036286426	T	T	T
0.0179794843649993	0.0009047992111282	0.5053573092892129	T	T	T

(3) PEA_2SnBr_4

2D-1-PEA2SnBr4

1.00000000000000

5.9394173067928859	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.9178420454127343	0.0000000000000000
0.0000000000000000	0.0000000000000000	40.0000000000000000

H	C	N	Br	Sn
24	16	2	4	1

Selective dynamics

Direct

0.7967757021362892	0.3829717384528588	0.3711379915980482	T	T	T
0.0636339521294676	0.7449043603176289	0.3372898054485618	T	T	T
0.2230614628736450	0.2243357758162828	0.3839746651315230	T	T	T
0.2423826372276636	0.9263824328790992	0.3818880190655874	T	T	T
0.5194460071386119	0.3775146409490801	0.3251470400021347	T	T	T
0.7844871625047264	0.7387489134689627	0.2912270096043689	T	T	T
0.9219336291223220	0.8937010789262849	0.4233528935396080	T	T	T
0.9056559650275228	0.1946470963384649	0.4252684034860389	T	T	T
0.5100775402957167	0.0557201839270901	0.2848815364145798	T	T	T
0.1360219022163129	0.0597123158254530	0.4700469538281950	T	T	T
0.2999747791796920	0.1991549704254687	0.4434755644100957	T	T	T
0.3004332932253461	0.9093298121932377	0.4443622387720886	T	T	T
0.2895561485769232	0.3654097118134778	0.6567371388607183	T	T	T
0.9891065610440961	0.7339788764805020	0.6868426876439326	T	T	T
0.8761350784208932	0.2092838259279013	0.6362735057725029	T	T	T

0.8527669000348154 0.9112580976721960 0.6385272774914716 T T T
0.5294944461749188 0.3604924995309892 0.7071713960297460 T T T
0.2295441844445045 0.7290836073733526 0.7375102265102136 T T T
0.2083866782404831 0.8722628112905489 0.6042383447410609 T T T
0.2317968250472688 0.1714139011116919 0.6023137624914998 T T T
0.5019784262325737 0.0426937698006036 0.7479454116001877 T T T
0.0581294297901818 0.0320227294745556 0.5534266651509645 T T T
0.8626464335211403 0.1805945610641068 0.5747660232968799 T T T
0.8552072432670055 0.8936916456743716 0.5749363006372110 T T T
0.9509301862066341 0.0638144052187593 0.3574751601962102 T T T
0.7956946542128428 0.2409846650191424 0.3536673597791699 T T T
0.9438366425769161 0.8839121445845708 0.3346899162691295 T T T
0.1234325702077297 0.0672407173299704 0.3852684184760731 T T T
0.6382971751300481 0.2379095834310030 0.3277330517477824 T T T
0.7866854974140310 0.8805496506876538 0.3086797488375456 T T T
0.0176105315549024 0.0510832064768095 0.4200677936640993 T T T
0.6331857106509060 0.0577607289677258 0.3051271355931249 T T T
0.1218576851378738 0.0491992455541984 0.6681450276852201 T T T
0.2754335889244145 0.2248002409195620 0.6743268026294188 T T T
0.1079997751486558 0.8716424110172518 0.6912567578278035 T T T
0.9744746444335750 0.0513058117707781 0.6373084922988482 T T T
0.4112940225389644 0.2223677944781664 0.7028160976703413 T T T
0.2432978126512761 0.8690404563333836 0.7198518364237286 T T T
0.1125194022108395 0.0308953354770688 0.6051759560915988 T T T
0.3956835576040684 0.0444199063690091 0.7256960868476270 T T T
0.1993496036486267 0.0543132733058892 0.4460478748215533 T T T
0.9616722960639057 0.0345001608551622 0.5750370230576340 T T T
0.4562402503489430 0.0254686238158193 0.5223709898583190 T T T
0.4848201382931853 0.5538582269918810 0.4383597103952644 T T T
0.6537807732267986 0.5363895001396501 0.5867281811817645 T T T
0.9869681339383025 0.4974692745790364 0.5036776996247818 T T T
0.5288379600044641 0.5279572799432922 0.5146600174957408 T T T

(4) $PEA_2CsSn_2Br_7$

2D-2-PEA2CsSn2Br7

1.00000000000000

5.9435065533034619 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.9252275770099629 0.0000000000000000
0.0000000000000000 0.0000000000000000 40.0000000000000000

H C N Br Sn Cs

24 16 2 7 2 1

Selective dynamics

Direct

0.8053707963145793 0.3729991062754755 0.2879669393663617 T T T

0.0685647580685690	0.7371183426393753	0.2530119430322573	T	T	T
0.2188382844647744	0.2094367582623756	0.3032258629516107	T	T	T
0.2459831923321865	0.9136861700187258	0.2984288058083414	T	T	T
0.5353371847587557	0.3783202674414698	0.2409956282369895	T	T	T
0.7971139073726690	0.7418031828099512	0.2059348441351733	T	T	T
0.9148568761265399	0.8556925161056944	0.3373578737664603	T	T	T
0.8913398960551998	0.1537370638894600	0.3422035601809416	T	T	T
0.5278394731491655	0.0627849538892540	0.1997217754551100	T	T	T
0.1109025655269677	0.9819759978245149	0.3867125336480998	T	T	T
0.2748173695478139	0.1580891622149303	0.3642886004209930	T	T	T
0.2928325163244173	0.8729904797968481	0.3597025523069082	T	T	T
0.2714401338361228	0.3722543536795306	0.7151998886533606	T	T	T
0.9930737519559810	0.7317376372259022	0.7453493780113160	T	T	T
0.8631347003458434	0.2052452358363688	0.6952179190341897	T	T	T
0.8465506786992429	0.9071135375218822	0.6975268671365162	T	T	T
0.5161379850137322	0.3727251129201869	0.7651268712336955	T	T	T
0.2383619843410181	0.7320652506036318	0.7955198051505059	T	T	T
0.1993552468481803	0.8748814209065856	0.6626481489093047	T	T	T
0.2184701768654340	0.1739928211179233	0.6608314955176269	T	T	T
0.5024935627221262	0.0527641883876004	0.8056265808463344	T	T	T
0.0429096302275323	0.0291247251010539	0.6120769574971717	T	T	T
0.8497879799854205	0.1795344678318004	0.6335632227304689	T	T	T
0.8418539224862167	0.8937469967209603	0.6341604060894688	T	T	T
0.9569512375659510	0.0542425212270916	0.2737864657531210	T	T	T
0.8051568978084515	0.2340618484862813	0.2699961151765961	T	T	T
0.9513329076753292	0.8780637396259150	0.2503995200891219	T	T	T
0.1230019693724495	0.0500898661495767	0.3024233942819129	T	T	T
0.6519354807668291	0.2369993913349281	0.2435262720349839	T	T	T
0.7984702302687958	0.8807780739408334	0.2238487549447396	T	T	T
0.0081344847998069	0.0156591274380054	0.3362990835112009	T	T	T
0.6479550385236182	0.0603402433300687	0.2203559370532405	T	T	T
0.1146868590002323	0.0510579302660422	0.7266847371586505	T	T	T
0.2632834539991424	0.2308425069858503	0.7327030884256212	T	T	T
0.1082465775192220	0.8724896158047348	0.7496566538785335	T	T	T
0.9649691134401793	0.0496752481269787	0.6961078045237579	T	T	T
0.4018660685341713	0.2313631982843375	0.7608926858461192	T	T	T
0.2462728621572417	0.8728456684382279	0.7779544023090902	T	T	T
0.1014132846854761	0.0319538879492221	0.6637882775890559	T	T	T
0.3939196936933941	0.0522387276935668	0.7836237748729714	T	T	T
0.1819534711115682	0.0087503842294836	0.3634879495512642	T	T	T
0.9485943981164365	0.0339658318591032	0.6338617665393211	T	T	T
0.5501010704248716	0.0645520897065635	0.4297020184314432	T	T	T
0.4486764647719146	0.0390093362059892	0.5801919633810809	T	T	T
0.4804930582276082	0.5252679976581628	0.3521596717942574	T	T	T

0.5050196127001509	0.5476173281183256	0.5007464693942305	T	T	T
0.6346699616173471	0.5402757734258423	0.6479006796396476	T	T	T
0.0405423147996331	0.5854668944500770	0.4267659330183175	T	T	T
0.9862921333348179	0.5421860478467363	0.5670292370579435	T	T	T
0.5357165704935906	0.5491212335258455	0.4267569017380374	T	T	T
0.5196766698399228	0.5412069346126074	0.5761736460660003	T	T	T
0.0558315413833829	0.0422548042581060	0.4986253358205083	T	T	T

(5) EA_2SnBr_4

2D-1-EA2SnBr4

1.00000000000000

5.8992667631655022	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.8597194547931943	0.0000000000000000
0.0000000000000000	0.0000000000000000	35.0000000000000000

H	C	N	Br	Sn
16	4	2	4	1

Selective dynamics

Direct

0.9651625217779988	0.1827778973864120	0.3616543811279002	T	T	T
0.9669094570541186	0.8780107351708832	0.3595989364780722	T	T	T
0.2157991152844506	0.0347926092726316	0.3480879457779169	T	T	T
0.2483997801017390	0.1698771056901704	0.4160851636601260	T	T	T
0.2482155916368203	0.8662244801786483	0.4140643775205863	T	T	T
0.8509586163350334	0.1618723826539739	0.4330969791057485	T	T	T
0.9989393519085247	0.9920317237928824	0.4629618528749759	T	T	T
0.8436500654761840	0.8718438270737991	0.4291058011943054	T	T	T
0.9662512211773097	0.8802354694982361	0.6563075324364344	T	T	T
0.9670735457459119	0.1849862458741802	0.6542853083804091	T	T	T
0.2140275769977595	0.0351337403510743	0.6691583384651191	T	T	T
0.2579710436169205	0.8669648179834528	0.6033610740355676	T	T	T
0.2596068017244930	0.1705072625384952	0.6013108676404028	T	T	T
0.8563799617904784	0.8737518069608972	0.5863180581579941	T	T	T
0.0178382959080848	0.9938357814020541	0.5532085373592490	T	T	T
0.8648240689711766	0.1634389498711239	0.5824045912158465	T	T	T
0.0676812763907753	0.0294622081607896	0.3670520183917743	T	T	T
0.1468533324023314	0.0197269157703210	0.4083155026473219	T	T	T
0.0694766807953546	0.0309626912783165	0.6494209581758354	T	T	T
0.1561384578626928	0.0208145183409255	0.6085900925422393	T	T	T
0.9478637739924696	0.0127769822469429	0.4349585364588491	T	T	T
0.9618945136927947	0.0144164620290068	0.5809492334855924	T	T	T
0.5579559843920164	0.0617953744227483	0.5090096995741817	T	T	T
0.6480276300899909	0.5204272973393653	0.4223589529811599	T	T	T
0.6587411649604531	0.5235917557505650	0.5939536552936986	T	T	T
0.0814248243182777	0.6056471913965201	0.5075403238836934	T	T	T

0.5933823455958480 0.5479237675655781 0.5083432811349924 T T T

(6) $EA_2CsSn_2Br_7$

2D-2-EA2CsSn2Br7

1.00000000000000

5.9311056395955157 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.8845065374536585 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

H C N Br Sn Cs

16 4 2 7 2 1

Selective dynamics

Direct

0.9244579144647684 0.1752859552673508 0.2698968596964983 T T T

0.9246024887632865 0.8714279097038707 0.2699915642237267 T T T

0.1570455422679579 0.0232488634220688 0.2504475344180965 T T T

0.2558838598238223 0.1751272295677439 0.3156094283869822 T T T

0.2561937200832822 0.8730864127099637 0.3157044507205424 T T T

0.8787206219529403 0.1683158904376250 0.3426487727478344 T T T

0.0639915675940918 0.0245301037629412 0.3699600768555857 T T T

0.8788622700076199 0.8799484490918161 0.3427402062440932 T T T

0.9242071061475006 0.8694000023951227 0.7229723126784777 T T T

0.9237021589287172 0.1732480080744468 0.7229373210491808 T T T

0.1549331486394316 0.0218079471242470 0.7429744952591737 T T T

0.2592643556316882 0.8707820381820309 0.6779885499421948 T T T

0.2587408377004119 0.1727883965443268 0.6779747200317662 T T T

0.8839694143360898 0.8771662009355112 0.6501299743692803 T T T

0.0715636966185998 0.0212144541555513 0.6232594333262698 T T T

0.8838652173986460 0.1654113948346539 0.6500958385191411 T T T

0.0305476449999291 0.0234478570390763 0.2733472515987331 T T T

0.1495594003587375 0.0239503202089577 0.3117685550445451 T T T

0.0302290159087566 0.0214924038537796 0.7197938942087352 T T T

0.1522089986351036 0.0216031010067669 0.6816393081130508 T T T

0.9815186093757269 0.0241621310520208 0.3439356459180123 T T T

0.9867470265390883 0.0212975358423417 0.6490861233300479 T T T

0.4939587203698896 0.0228741984090694 0.4071811078894614 T T T

0.4939688311958778 0.0204064890185409 0.5862322979857295 T T T

0.6675379238511397 0.5232719259560905 0.3276880800833079 T T T

0.5326262628457074 0.5218234151278492 0.4965645701405320 T T T

0.6710956779643187 0.5205629026873381 0.6653707720774825 T T T

0.0244414045211029 0.5219997501225957 0.4200448322606266 T T T

0.0250232476231277 0.5200598234229464 0.5726834222793891 T T T

0.5547965129819753 0.5222852869664293 0.4107197916566467 T T T

0.5563116546213882 0.5202969383730611 0.5824968792935752 T T T

0.0808721478492848 0.0215056647038483 0.4964139296512822 T T T

(7) DMA_2SnBr_4

2D-1-DMA2SnBr4

1.00000000000000

6.0325164524987320 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.9966964251188637 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

H C N Br Sn

16 4 2 4 1

Selective dynamics

Direct

0.8000541118858556	0.8856961184068196	0.4479351306025577	T	T	T
0.8026639438943659	0.1870269507023872	0.4474658108459894	T	T	T
0.9307971021432931	0.0372495187517164	0.4858265497101873	T	T	T
0.9903395892925601	0.1827887330393300	0.3834248536261930	T	T	T
0.9868600316540723	0.8824140710942878	0.3837291799086694	T	T	T
0.2439651996457371	0.0293464673191719	0.3782571489316855	T	T	T
0.2000089165751459	0.8910257762061495	0.4415955538791855	T	T	T
0.2025961446205675	0.1734533724359087	0.4414074843587228	T	T	T
0.0038708079303744	0.8904177595657168	0.6629985113518349	T	T	T
0.0076374173780367	0.1909460762134682	0.6625826779070069	T	T	T
0.2621859913205201	0.0376393013751397	0.6659416397039284	T	T	T
0.8020040429388446	0.1901022082775866	0.6000435078134755	T	T	T
0.7994083272516294	0.8886671941328287	0.6002771620373382	T	T	T
0.9195638219269594	0.0372709004742480	0.5610569007021732	T	T	T
0.2007839826614770	0.8946823867630204	0.6034028068397153	T	T	T
0.2032358753346449	0.1767997398542121	0.6030123550886100	T	T	T
0.8944605342454308	0.0359464251924226	0.4552383081025155	T	T	T
0.0803121224724185	0.0318145957313372	0.3917934563905945	T	T	T
0.0948559806944298	0.0391365783576408	0.6538139794925391	T	T	T
0.8917102390777372	0.0383803980251067	0.5919082306560731	T	T	T
0.1088392533111788	0.0329295760096013	0.4339451943128846	T	T	T
0.1115532314639345	0.0369778550558591	0.6114771401342092	T	T	T
0.4047399989134743	0.0558510956933977	0.5229016362330675	T	T	T
0.3762854344563943	0.5330966481619986	0.4353654897582937	T	T	T
0.3796157116814454	0.5370043451630384	0.6099567930570367	T	T	T
0.9409968246028841	0.5404680630207364	0.5233963109644019	T	T	T
0.3961743626265957	0.5321238449768885	0.5228091875911345	T	T	T

(8) $DMA_2CsSn_2Br_7$

2D-2-DMA2CsSn2Br7

1.00000000000000

6.0339244899779292 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.9922279260461861 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

H C N Br Sn Cs

16 4 2 7 2 1

Selective dynamics

Direct

0.8184028898307548 0.8794712094682424 0.3574848781346065 T T T

0.8206964902137569 0.1805816809905580 0.3573666424448474 T T T

0.9556619297519212 0.0294985228023396 0.3949387830703663 T T T

0.9985933736252341 0.1804002610580160 0.2923618604668705 T T T

0.9931844323680665 0.8796288710298137 0.2923218283100758 T T T

0.2500707829522535 0.0253952725581045 0.2857768068644823 T T T

0.2168350203243835 0.8848965280166358 0.3490712334061353 T T T

0.2192533932179905 0.1681636115937225 0.3492043959049537 T T T

0.9731516634187688 0.8792932749731877 0.7353117961202882 T T T

0.9760628170198882 0.1798506105549013 0.7354219097538605 T T T

0.2259142916006249 0.0269817448259101 0.7448364297860236 T T T

0.8236497972005457 0.1810539696440732 0.6688204552652922 T T T

0.8225206853443170 0.8800371702682869 0.6684904937116233 T T T

0.9725210619265880 0.0313691010753930 0.6326570143180017 T T T

0.2169207054244520 0.8864323522683812 0.6810987849177825 T T T

0.2184707920343360 0.1701354442326580 0.6811422926400712 T T T

0.9141458798840225 0.0293922011623686 0.3645312113211997 T T T

0.0887562971768275 0.0282876960613250 0.3001097618912028 T T T

0.0704927327362323 0.0287153539269401 0.7286765998219359 T T T

0.9200041208272691 0.0304043414433509 0.6625535262544652 T T T

0.1245086171462251 0.0274911597345145 0.3421030848158471 T T T

0.1219847878412882 0.0287628314651596 0.6871705055332707 T T T

0.4280417395491654 0.0516026819706461 0.4317951100505220 T T T

0.4327737191489640 0.0520316831710797 0.5967225671488549 T T T

0.3850317991998197 0.5277502825329724 0.3425943855500257 T T T

0.4635909507966200 0.5404775225952421 0.5145897075660282 T T T

0.3826045829912409 0.5282550017657622 0.6868020569967640 T T T

0.9629478169833833 0.5342168553326039 0.4380425301239830 T T T

0.9658315792082199 0.5342939179175870 0.5904707248626095 T T T

0.4201517679044975 0.5254317228162214 0.4311441023085072 T T T

0.4224484496270726 0.5254417139719918 0.5978961301065041 T T T

0.9302910327252930 0.0335084087720090 0.5145673905330185 T T T

(9) MA_2SnBr_4

2D-1-MA2SnBr4

1.00000000000000

5.8471511128002405 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.8453691645863950 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

H C N Br Sn
12 2 2 4 1
Selective dynamics
Direct
0.0034093596543933 0.0403360333666070 0.4744630150762991 T T T
0.2124396465672586 0.8931492303477950 0.4516970575590508 T T T
0.2132718578705058 0.1844606407847176 0.4512688471146499 T T T
0.8583146409703697 0.1910423415953239 0.4150172091972629 T T T
0.0791982916288980 0.0357028797902568 0.3904021374881430 T T T
0.8577391146523389 0.8843760398983694 0.4155117048781290 T T T
0.9005443990144891 0.2057268519511031 0.5942616465092225 T T T
0.1918582179015676 0.2069045312685653 0.5946074457533504 T T T
0.0478174464164242 0.9978191362217621 0.5712403914182197 T T T
0.8927146339530136 0.8493942760846256 0.6300296142848176 T T T
0.1993478315131204 0.8505497634998510 0.6304792721871277 T T T
0.0436771398347552 0.0701318996271200 0.6553848888057539 T T T
0.9657964378796019 0.0375173441166713 0.4152865291617493 T T T
0.0456350610325178 0.9577207861986939 0.6303675257757164 T T T
0.1085884377988440 0.0391682635135509 0.4505265261196266 T T T
0.0467391463183448 0.1020539663890227 0.5952912156210682 T T T
0.6262041745491437 0.0665550041540915 0.5095149112692775 T T T
0.4118255439144466 0.5418803977648733 0.4398761340536133 T T T
0.5502879102532208 0.4046720247506260 0.6059094663802193 T T T
0.0743203922417027 0.6187386540867019 0.5363220840242969 T T T
0.5508193160350383 0.5432589345896716 0.5228923773224072 T T T

(10)$MA_2CsSn_2Br_7$

2D-2-MA2CsSn2Br7
1.00000000000000
5.9412572164750301 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.9790832556709521 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000
H C N Br Sn Cs
12 2 2 7 2 1
Selective dynamics
Direct
0.9007015890567643 0.9790005684494634 0.3545990746293433 T T T
0.1839387334214815 0.9862932084574343 0.3539463683587847 T T T
0.0356900363715515 0.2209606702209291 0.3500467064610869 T T T
0.8817550827528228 0.1029708701721681 0.2885017708636450 T T T
0.1844505734861308 0.1120465099229135 0.2877804919364371 T T T
0.0414624543362176 0.8480225278472212 0.2926549820163531 T T T
0.8977748214840511 0.2601177726308289 0.6489522546889374 T T T
0.1872856928128646 0.2607689707872073 0.6497984772111071 T T T

0.0471561568165280 0.1492755888363206 0.6135843331395145 T T T
0.8921347154952397 0.8531680154471691 0.6545790005841370 T T T
0.1949569386159201 0.8549988959333295 0.6556231152455144 T T T
0.0379981630602880 0.9787788908039057 0.6939174427548639 T T T
0.0364856932999014 0.0266789743778844 0.2994360332114990 T T T
0.0420135689780059 0.9476356793039752 0.6630908007399258 T T T
0.0393852090247999 0.0534692672232558 0.3417676478344592 T T T
0.0432973028661601 0.1670121419821738 0.6429213397230856 T T T
0.5379918083335199 0.9906024118348341 0.3936757025594635 T T T
0.5036332401442879 0.0099690667212528 0.5650714049780599 T T T
0.5282172268462100 0.4878669409657320 0.3139911969645474 T T T
0.5293185779628923 0.4979905538275360 0.4842068857871633 T T T
0.5409939704256370 0.4369133249136519 0.6550574170070476 T T T
0.0306356211643439 0.5242511982414180 0.3959669753907997 T T T
0.0133464389157173 0.4909947335365884 0.5633982166391429 T T T
0.5305917166178494 0.5020525951655879 0.3925842937799150 T T T
0.5229271977142123 0.4904846313193637 0.5672459564463646 T T T
0.9964104699965941 0.9888399910778777 0.4908871110488002 T T T

(11)PMA_2SnBr_4

2D-1-PMA2SnBr4

1.00000000000000

5.9684823501332636 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.9361416952826254 0.0000000000000000
0.0000000000000000 0.0000000000000000 40.0000000000000000

H C N Br Sn
20 14 2 4 1

Selective dynamics

Direct

0.9327888426043051 0.9587474173944239 0.2911638136028443 T T T
0.1578277458206422 0.6785854874182514 0.3233690050278828 T T T
0.2141137924799191 0.7286245612737550 0.3844442085379566 T T T
0.8239597984243699 0.3408415648692646 0.3813102541053845 T T T
0.7659284427831592 0.2892886336234053 0.3205544018865660 T T T
0.1355675323145338 0.2276588158173692 0.4301882208372356 T T T
0.1681252569648050 0.9305802694312456 0.4338005553456358 T T T
0.7417013701960575 0.1925678161949332 0.4392606833573084 T T T
0.8716361501726305 0.0447829140422883 0.4689236452133029 T T T
0.7522250230614402 0.9050091274712230 0.4377200998878658 T T T
0.0674346429324701 0.9555123720002762 0.7292833065189488 T T T
0.8441197640969172 0.6745492767361516 0.6969617169465340 T T T
0.7870816164342546 0.7256989247656013 0.6359030853207343 T T T
0.1723829792779293 0.3409237413027491 0.6393514989678523 T T T
0.2312071527932427 0.2883087242811856 0.7000680653000881 T T T

0.8647672554194292 0.2261527261600325 0.5902025414451958 T T T
0.8347387520015370 0.9283844760259176 0.5864181178238683 T T T
0.2604914894906725 0.1927383097412627 0.5822339064396380 T T T
0.1349004079830432 0.0488546890209593 0.5519058766063700 T T T
0.2493848096212570 0.9048902091150161 0.5831019598375542 T T T
0.9579738968174649 0.9805237822599054 0.3179985847303164 T T T
0.0839995934902335 0.8236646917805659 0.3359947162458142 T T T
0.1150199471856894 0.8509923894976965 0.3703761305612988 T T T
0.0216597439512223 0.0363971883767179 0.3870133197958957 T T T
0.8968154748913274 0.1945861032028711 0.3687437605849363 T T T
0.8643008783415268 0.1658170702877949 0.3344509348717335 T T T
0.0590484307565631 0.0642327365441761 0.4240878633033178 T T T
0.0416219363114176 0.9779373961333179 0.7024739325917295 T T T
0.9166117240018868 0.8205973745044237 0.6844080207943020 T T T
0.8851530647353292 0.8485428863741716 0.6500408903422982 T T T
0.9771209419540803 0.0350255253278765 0.6334953331972123 T T T
0.1006707906750444 0.1938047794802272 0.6518473475338189 T T T
0.1336029967295045 0.1644936050813553 0.6861194426852955 T T T
0.9416892508560555 0.0629972080432294 0.5963808082627112 T T T
0.8428375473479733 0.0514372117340410 0.4434756185485046 T T T
0.1597660584627096 0.0520064518311227 0.5774950578348360 T T T
0.4728213811714472 0.0923451840749283 0.5077249316660432 T T T
0.5541208744474088 0.5569749051965572 0.4348738424356788 T T T
0.4499577033143555 0.5547604031115076 0.5847762161484549 T T T
0.9674580081370004 0.6309039024814873 0.5128264705246629 T T T
0.4955789315491288 0.5788821479907076 0.5097058143323779 T T T

(12)$PMA_2CsSn_2Br_7$

2D-2-PMA2CsSn2Br7

1.00000000000000

5.9668133586384702 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.9444272745386444 0.0000000000000000

0.0000000000000000 0.0000000000000000 40.0000000000000000

H C N Br Sn Cs

20 14 2 7 2 1

Selective dynamics

Direct

0.9432748314639784 0.9406235399486798 0.2064195989751207 T T T
0.1553249013518468 0.6622939933968294 0.2408134111060890 T T T
0.1980171665151774 0.7211637879169555 0.3019394105060665 T T T
0.8212948533056598 0.3393843940309199 0.2945560094107358 T T T
0.7770679149184845 0.2792667487044726 0.2336789697405613 T T T
0.1088534392602843 0.2301064903654167 0.3457800818407171 T T T
0.1444220543846175 0.9340360201789356 0.3504573180585536 T T T

0.7127310650125520	0.1896548394730376	0.3514865292661986	T	T	T
0.8315423395289164	0.0557235896045830	0.3831538455071778	T	T	T
0.7293062095283780	0.9021201067691176	0.3518571590626608	T	T	T
0.0566112827437309	0.9348306859261588	0.7903377397124293	T	T	T
0.8449686323502457	0.6568697466193161	0.7558155137336324	T	T	T
0.8008453295337927	0.7178156514507235	0.6947586012041265	T	T	T
0.1756827322574324	0.3370335839504008	0.7024550378061771	T	T	T
0.2214215333445241	0.2748000580853600	0.7632652277397518	T	T	T
0.8881101830172673	0.2285678616324836	0.6512110413629526	T	T	T
0.8526344268230071	0.9325513497888273	0.6463923549227930	T	T	T
0.2841831656916233	0.1883333040279717	0.6454194427952449	T	T	T
0.1653641714587733	0.0547663291781704	0.6137111508910804	T	T	T
0.2677109615154403	0.9008667967836012	0.6449775043200410	T	T	T
0.9626725439208254	0.9665000484754935	0.2332864744687396	T	T	T
0.0811973931022767	0.8105395209871465	0.2525136117149838	T	T	T
0.1044009820399843	0.8427900035478966	0.2869444906489752	T	T	T
0.0105387757616689	0.0321968683687598	0.3024299493138157	T	T	T
0.8938862769432453	0.1897842296438877	0.2829029722428914	T	T	T
0.8692137638507790	0.1562272555447017	0.2485542821778698	T	T	T
0.0368012449024443	0.0648900299227732	0.3396482183184012	T	T	T
0.0366327348615280	0.9615446803104180	0.7634984014466626	T	T	T
0.9182658960638271	0.8058454426035645	0.7442046310181896	T	T	T
0.8942641063788623	0.8392602726594265	0.7098116386525195	T	T	T
0.9870853429795260	0.0295791831706493	0.6944352118414322	T	T	T
0.1037173914121280	0.1868357366331089	0.7140244345176376	T	T	T
0.1292272264444933	0.1520925621260103	0.7483343932829205	T	T	T
0.9602559865419142	0.0632396051027530	0.6572462922357205	T	T	T
0.8144880083840887	0.0517042781568497	0.3574106810972845	T	T	T
0.1824630966184578	0.0504792903637882	0.6394524566375339	T	T	T
0.5041756246384609	0.0745763180534242	0.4283329476477363	T	T	T
0.4921087960191093	0.0745972991899340	0.5685224279953386	T	T	T
0.5362183191416707	0.5493703638875099	0.3491685865586662	T	T	T
0.4975352195995930	0.5696459225924043	0.4985525385458658	T	T	T
0.4607508591152125	0.5486517973275747	0.6479291543172735	T	T	T
0.9814305514343368	0.5745821358793906	0.4252853400327559	T	T	T
0.0157966763361735	0.5746257477520237	0.5719352633007346	T	T	T
0.5035894687687313	0.5600264820470899	0.4245411532908805	T	T	T
0.4931625664296648	0.5595040717884417	0.5726121734556322	T	T	T
0.9989659543052777	0.0497309760330108	0.4984443272774294	T	T	T

(13)GA_2SnBr_4

2D-1-GA2SnBr4

1.00000000000000

6.3506940929269486 0.0000000000000000 0.0000000000000000

0.0000000000000000 6.3390114115082943 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000
H C N Br Sn
12 2 6 4 1
Selective dynamics
Direct
0.2790351526427262 0.2519380546435647 0.4146621172917422 T T T
0.7504404357690367 0.1521801040363754 0.4431868616780556 T T T
0.9550923619368185 0.3266409495877140 0.4454218269705295 T T T
0.8036781647606422 0.8113636745120894 0.4143721804060294 T T T
0.0571798153724144 0.7533096953163092 0.3986232236776287 T T T
0.3217572154565845 0.9886923826805124 0.4015504437725746 T T T
0.3219723012646817 0.9923042743743569 0.6016301200632115 T T T
0.8039328921579048 0.8183554563098151 0.5872560256335299 T T T
0.0559928973382512 0.7578861104674819 0.6034360201551607 T T T
0.7545736204883429 0.1605983320142977 0.5589120928075236 T T T
0.9603053496947648 0.3339060424569006 0.5573652005642067 T T T
0.2813783757706150 0.2564605566753937 0.5888894245672242 T T T
0.0199522084835705 0.0559614702225265 0.4159313296706741 T T T
0.0216009028645166 0.0618423399419803 0.5866502442856838 T T T
0.2185406325633895 0.1081507684986814 0.4072626563164046 T T T
0.8913404470795251 0.1984997817206940 0.4319923193918933 T T T
0.9488561933299292 0.8643086330820353 0.4061714930984360 T T T
0.2196701018489934 0.1126128636592555 0.5959629462529840 T T T
0.9488684719788136 0.8698995997212818 0.5958220518056431 T T T
0.8948023341368635 0.2059035094694844 0.5705537644438431 T T T
0.4850540811464055 0.1755430802649611 0.5015789480152486 T T T
0.4502848728789694 0.6144837770152765 0.4154505080251973 T T T
0.4488167752508045 0.6176879367735406 0.5869776158147866 T T T
0.0127878712325475 0.5941142940593315 0.5008645958104330 T T T
0.4455005245529015 0.6118293124961495 0.5012269894813419 T T T

(14)$GA_2CsSn_2Br_7$

2D-2-GA2CsSn2Br7
1.00000000000000
6.2600910762022171 0.0000000000000000 0.0000000000000000
0.0000000000000000 6.2548102454760954 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000
H C N Br Sn Cs
12 2 6 7 2 1
Selective dynamics
Direct
0.1902336802542932 0.3443747692888037 0.3179870610757214 T T T
0.0479489636121469 0.8240264200261055 0.3515874135809009 T T T

0.2428844896097227	0.0167952562384867	0.3516790113028844	T	T	T
0.7226155077944314	0.8804542753655489	0.3175606592929520	T	T	T
0.6748643567325221	0.1416827934771925	0.3018780083246990	T	T	T
0.9303485763508196	0.3946774839994973	0.3019865970705853	T	T	T
0.3629571368036612	0.9549341261508958	0.6709158458823942	T	T	T
0.8497367637359577	0.7499095466786423	0.6552268812151407	T	T	T
0.1097562744632398	0.7019206610359401	0.6710660045696870	T	T	T
0.7867810651028686	0.0852082972438825	0.6238695962440944	T	T	T
0.9802898420487958	0.2781448335219501	0.6237597496508205	T	T	T
0.3149535682644665	0.2150706821372203	0.6550770893951414	T	T	T
0.9771515348743823	0.0912086736947206	0.3205322607998378	T	T	T
0.0591527791448761	0.0058362631181685	0.6533661640789392	T	T	T
0.0427808293257350	0.2871756054444952	0.3106392681565522	T	T	T
0.1102374726705377	0.9561612164824524	0.3385284353277944	T	T	T
0.7812489901197637	0.0276318046638883	0.3103082433619221	T	T	T
0.2555316908300500	0.0698324663087659	0.6633112967942555	T	T	T
0.9951406719303209	0.8093243697517279	0.6633318604089730	T	T	T
0.9245482909107893	0.1406851950803935	0.6358185206034880	T	T	T
0.5014493303461800	0.1047122258496383	0.4074697904471608	T	T	T
0.5003343562068016	0.1155291752706105	0.5662338070560368	T	T	T
0.5419316495713570	0.5283478518572641	0.3161455640687139	T	T	T
0.4563896783967941	0.5861315951954432	0.4853320039824137	T	T	T
0.4992951362448829	0.5662652834639432	0.6549851709103333	T	T	T
0.9611961948311134	0.5674658530757786	0.4086023829750021	T	T	T
0.9510844442213093	0.5635066100077464	0.5655713610886751	T	T	T
0.5231880407536136	0.5454079854223713	0.4021865783175536	T	T	T
0.5074205925804053	0.5604527424889584	0.5685971944258260	T	T	T
0.0499660922681722	0.0816029376594593	0.4869111795915161	T	T	T

(15)BA_2SnBr_4 (R-P-1)

R-P-1-BA2SnBr4-

1.00000000000000

11.5547229662599484	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7565175579688823	0.0000000000000000
0.0000000000000000	0.0000000000000000	34.5359191894531250

H	C	N	Br	Sn
96	32	8	16	4

Selective dynamics

Direct

0.9964367818145277	0.8340276427327480	0.8916315427978305	T	T	T
0.9920905314022479	0.1403830808540801	0.8969972185019426	T	T	T
0.1079427127739822	0.8767983691375729	0.8296477183425133	T	T	T
0.1059354369599132	0.1838716961035444	0.8347880586990406	T	T	T
0.8967413985126843	0.8810645021543397	0.8265612870113226	T	T	T

0.9553146774665270	0.0525472025109088	0.7923732141382112	T	T	T
0.2085470166150392	0.1537043103670964	0.8995609262207981	T	T	T
0.2152232729545530	0.8502989382491241	0.8926460560797639	T	T	T
0.1105785833015044	0.7865715914895487	0.9560456575156213	T	T	T
0.1024944823667751	0.0915540234007795	0.9630807986337805	T	T	T
0.2389838478191587	0.9507376079994055	0.9630428414063023	T	T	T
0.8958111854952251	0.1756452111236181	0.8307967697441577	T	T	T
0.4459226217696760	0.9130316621302218	0.9021107883941862	T	T	T
0.4180955223389521	0.2014592632201641	0.8870143296936998	T	T	T
0.6110559559601750	0.8835649861546647	0.8559263487711670	T	T	T
0.6046505199116777	0.1873400926487713	0.8467582279363931	T	T	T
0.4196868173563804	0.8438377111673746	0.8259524978539939	T	T	T
0.5141737578206216	0.9755859551202096	0.7961265916762048	T	T	T
0.6160105061074799	0.3195975156775402	0.9126901634518956	T	T	T
0.6306623487681233	0.0402204158285313	0.9330470529237820	T	T	T
0.4474903981785175	0.1067030847916226	0.9724658058953406	T	T	T
0.4340157711317473	0.3868625312763368	0.9515166434378625	T	T	T
0.5529042192229449	0.3227918404120683	0.9824120203548585	T	T	T
0.4137617387037231	0.1344487510934091	0.8192029516993482	T	T	T
0.5252887197760560	0.8286487782591709	0.6082289091377809	T	T	T
0.5312568551398524	0.1353400328129381	0.6039364119069366	T	T	T
0.4128237787358967	0.8645640802654030	0.6700000005980470	T	T	T
0.4166030326333622	0.1734900570034812	0.6661278831995292	T	T	T
0.6243735279644924	0.8652502555712600	0.6726460111559280	T	T	T
0.5670283471599793	0.0218133038047723	0.7082318039535780	T	T	T
0.3153112938006955	0.1531426362990662	0.5995119150736011	T	T	T
0.3066134892441661	0.8492783857641233	0.6061142406871053	T	T	T
0.4159083906612236	0.7842337248235945	0.5437650583753708	T	T	T
0.4251128821467667	0.0893076447484536	0.5366314202802410	T	T	T
0.2883015873532511	0.9490582557293806	0.5357775818266186	T	T	T
0.6252577759033434	0.1616043398070372	0.6710944497364090	T	T	T
0.0185179529165106	0.8533872708579051	0.6065265959526729	T	T	T
0.0222875853395955	0.1614160334874125	0.6065964982651911	T	T	T
0.9147924142686430	0.8562826478909611	0.6704784169280316	T	T	T
0.9168688505837450	0.1666657236207627	0.6704597369254288	T	T	T
0.1251310513616722	0.8570743412598709	0.6707880381798518	T	T	T
0.0755522152614047	0.0121445635526829	0.7079295468145094	T	T	T
0.8046517429495110	0.1715513713421139	0.6067988763538198	T	T	T
0.8010058824702233	0.8645033197942316	0.6064885906124003	T	T	T
0.9033347453277610	0.8612598937107233	0.5416401738233401	T	T	T
0.9069964939268779	0.1696357309000638	0.5419329707618317	T	T	T
0.7724392582736928	0.0216794726351466	0.5392910983935852	T	T	T
0.1271370886929248	0.1543967474129167	0.6700427763104622	T	T	T
0.1824947534773382	0.8532407298242579	0.3927609032298182	T	T	T

0.1563509351314736	0.1481337085963061	0.3811111905168382	T	T	T
0.3498085998023158	0.8416068173136837	0.3472039513446330	T	T	T
0.3415248879117512	0.1475286965093602	0.3403901965750450	T	T	T
0.1569483723315531	0.8075861954808704	0.3179909646895773	T	T	T
0.2514998221709402	0.9412387422198876	0.2883396510813412	T	T	T
0.3514573114275484	0.2554387664509640	0.4088410418675403	T	T	T
0.3707078202445769	0.9655160379291540	0.4240240074614950	T	T	T
0.1909084813740843	0.9945854577144211	0.4657400692585939	T	T	T
0.1693928320961421	0.2841353948845350	0.4495660357222259	T	T	T
0.2921325878443982	0.2140374083731708	0.4783142212266170	T	T	T
0.1519916769205439	0.0988454456346071	0.3121525490271421	T	T	T
0.7264623320588299	0.8092517184950373	0.3892730528064477	T	T	T
0.7243393909940623	0.1170113683871243	0.3918693412750041	T	T	T
0.8500101100228650	0.8294970149626160	0.3293341135627571	T	T	T
0.8494384474056791	0.1378200243108239	0.3319531286570097	T	T	T
0.6406161995079037	0.8367920466011943	0.3212469854746006	T	T	T
0.7062454380887649	0.0010124690435671	0.2875768130629409	T	T	T
0.9411100284550620	0.1212385433393612	0.3982669046160078	T	T	T
0.9439724735927529	0.8154143106781470	0.3953908285708066	T	T	T
0.8266551367981309	0.7887193847591638	0.4572224431756594	T	T	T
0.8227889212947748	0.0966048328807160	0.4600119043449057	T	T	T
0.9564408833859239	0.9477789544418067	0.4646555537947170	T	T	T
0.6395586419801197	0.1317968158528091	0.3241430375391181	T	T	T
0.7630260608244730	0.7808939342651290	0.1029362356084507	T	T	T
0.7702657825342104	0.0867795458464062	0.0974712835435330	T	T	T
0.6539534856066117	0.8255949565572079	0.1649223555893182	T	T	T
0.6572399774338151	0.1344204406131227	0.1599506820915734	T	T	T
0.8657044505500784	0.8276418050985874	0.1662812942356022	T	T	T
0.8110249973474541	0.9902600725071637	0.2017538427387678	T	T	T
0.5549746629234884	0.1093052008638745	0.0930320644827819	T	T	T
0.5438405089087777	0.8073780855988122	0.1015892519469425	T	T	T
0.6508460844002700	0.7232934724339583	0.0396049176091531	T	T	T
0.6635620074381346	0.0259065824110372	0.0303816559158600	T	T	T
0.5251670652633386	0.8924127801466228	0.0306173085207076	T	T	T
0.8659532023682359	0.1245611445125891	0.1636824204403567	T	T	T
0.2586990663634154	0.8163861324241182	0.1008976283692992	T	T	T
0.2618689763554101	0.1244406427868395	0.1009631145072952	T	T	T
0.1561762386706707	0.8192156773885408	0.1652602010982824	T	T	T
0.1591595449882761	0.1291480263921174	0.1653007973259878	T	T	T
0.3668934679633313	0.8181988121902098	0.1648773684419815	T	T	T
0.3171438265110615	0.9676641810501857	0.2023831249332352	T	T	T
0.0442109161116720	0.1325544601874687	0.1022501039275182	T	T	T
0.0413141909275560	0.8254504999550226	0.1019720731091610	T	T	T
0.1406699369643355	0.8235095118053113	0.0365999923179233	T	T	T

0.1434778613182705	0.1318181072263705	0.0369579686150730	T	T	T
0.0092079991027492	0.9824226482284651	0.0349632378849701	T	T	T
0.3691918303800975	0.1151610330528165	0.1649912159865192	T	T	T
0.0445684192566591	0.9955926574870746	0.8855260866563335	T	T	T
0.0594269449682280	0.0231146919030063	0.8420375823641010	T	T	T
0.1626320560428893	0.9898050809078723	0.9056494500231375	T	T	T
0.1532162105758706	0.9526832257822387	0.9492627223964364	T	T	T
0.4879266734099983	0.0751576540755688	0.8924864896070631	T	T	T
0.5527981103587033	0.0344191569765819	0.8547151058818401	T	T	T
0.5663057726603179	0.1718866678071251	0.9244173673656174	T	T	T
0.4966785933233901	0.2513399409149063	0.9596751858885559	T	T	T
0.4775574490342368	0.9903021132331902	0.6146886704318020	T	T	T
0.4618492647801719	0.0122723318766107	0.6582702379656188	T	T	T
0.3607862863681484	0.9882973493112388	0.5937094480494819	T	T	T
0.3731441783562382	0.9508751225098219	0.5501300858306755	T	T	T
0.9708767939651153	0.0097594699509479	0.6159715980829350	T	T	T
0.9614578140687833	0.0102195446373462	0.6599474211713811	T	T	T
0.8515092242094743	0.0160663819921162	0.5966939235875673	T	T	T
0.8589147021926877	0.0172682841932216	0.5525463263003068	T	T	T
0.2254531259294008	0.0182364747875252	0.3851570021283658	T	T	T
0.2906519473481419	0.9912344002050122	0.3471440560727960	T	T	T
0.3042486716723483	0.0984947481851944	0.4181569069641148	T	T	T
0.2356922395562624	0.1506976404417342	0.4550107584202294	T	T	T
0.7773010181591576	0.9669150794610986	0.3827889699624317	T	T	T
0.8004380867070229	0.9805506058435015	0.3395035450349074	T	T	T
0.8913227706151464	0.9634967768352044	0.4054278441134306	T	T	T
0.8733644036777999	0.9482354756184108	0.4491519049920643	T	T	T
0.7162035598357277	0.9442295691289234	0.1089193578065046	T	T	T
0.7023210303447426	0.9722653197091532	0.1525193672418095	T	T	T
0.5989294791824754	0.9416522288026402	0.0882164258048534	T	T	T
0.6102080192067383	0.8934089192137086	0.0448689854920705	T	T	T
0.2111300161611732	0.9723842031143972	0.1105771722975512	T	T	T
0.2030017980234240	0.9724561105248305	0.1545465187655574	T	T	T
0.0909240565111231	0.9774983493471081	0.0919096612708327	T	T	T
0.0963002188358561	0.9788784134201307	0.0477737515145814	T	T	T
0.9449969708330337	0.0323738162294585	0.8218179639018339	T	T	T
0.4698833819985872	0.9938533401909346	0.8219552964258877	T	T	T
0.5762181851903235	0.0153006938799099	0.6785120933769938	T	T	T
0.0788745299226458	0.0076588202197385	0.6780796911755921	T	T	T
0.2076030715777169	0.9571876819614361	0.3142641947931463	T	T	T
0.6900098816276593	0.9869411681336191	0.3168144039223716	T	T	T
0.8177337882338163	0.9785140398482658	0.1720212249340506	T	T	T
0.3207365342268969	0.9679742974652131	0.1724796719259004	T	T	T
0.2520397237082099	0.0066824018072892	0.7547545187738152	T	T	T

0.2226642509823313	0.5062082045771884	0.6622910654565854	T	T	T
0.3060882302917939	0.5090820819061246	0.8347653083892292	T	T	T
0.9921854063347813	0.4735966035464812	0.7483804159499814	T	T	T
0.7200494139467435	0.0180888404730708	0.7618759668978566	T	T	T
0.7323387462910813	0.5141853818025285	0.6668163489041296	T	T	T
0.7938182680882874	0.5289530466496760	0.8409889669795308	T	T	T
0.4937040879948164	0.5138357085393599	0.7408733585625386	T	T	T
0.4635991504580862	0.9743689209849983	0.2563119311472926	T	T	T
0.4731144393617465	0.4660696582227249	0.1603449536224517	T	T	T
0.5354864336083729	0.4840211553557370	0.3348059768019892	T	T	T
0.2337990487814958	0.4744278110728054	0.2366312355308677	T	T	T
0.9823704392221283	0.9697131947943630	0.2508170399357202	T	T	T
0.9630529969929602	0.4771759199136349	0.1582128436258967	T	T	T
0.0443849249926956	0.4740001498322787	0.3304342665498072	T	T	T
0.7325948131858443	0.4398763021156739	0.2426071640845575	T	T	T
0.2544165116607450	0.5069997113486086	0.7506224493509918	T	T	T
0.7496081887459515	0.5134504102367068	0.7541348912454903	T	T	T
0.4905630083031470	0.4701405505348164	0.2485595811978806	T	T	T
0.9932233458835451	0.4719878649371597	0.2461107024992368	T	T	T

(16)$BA_2CsSn_2Br_7$ (R-P-2)

R-P-2-BA2CsSn2Br7

1.00000000000000

11.5739939831386796	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.7764081252161681	0.0000000000000000
0.0000000000000000	0.0000000000000000	45.9260406494140625

H	C	N	Br	Sn	Cs
96	32	8	28	8	4

Selective dynamics

Direct

0.9098888778440433	0.8543940876042836	0.9167104950982894	T	T	T
0.9169036465155875	0.1604623859438965	0.9177658190034794	T	T	T
0.0915633055586916	0.8451350213010760	0.8860125571921911	T	T	T
0.0953853101725146	0.1533346378923499	0.8864563189193109	T	T	T
0.9032059423408355	0.8632349953272588	0.8631552835757724	T	T	T
0.0017412271650761	0.0100273588458849	0.8435372694802720	T	T	T
0.1087010620075293	0.1352671643848985	0.9437383214302684	T	T	T
0.1010939263602886	0.8303789583413939	0.9425484785607134	T	T	T
0.9155708742432452	0.8419446160481963	0.9720809638566156	T	T	T
0.9246977856829248	0.1481552997462108	0.9735473369106343	T	T	T
0.0306967433450637	0.9761903720720597	0.9912037551927357	T	T	T
0.9046944493728036	0.1550157443777125	0.8638611935731487	T	T	T
0.4113824495246962	0.8553942148573649	0.9170212979302842	T	T	T
0.4176408426301677	0.1616308863835369	0.9176516693142566	T	T	T

0.5919899504052162	0.8450934553154422	0.8859933670166747	T	T	T
0.5957944557538041	0.1532963829748488	0.8861819074094002	T	T	T
0.4029891739064026	0.8620278192499580	0.8634157933972545	T	T	T
0.5011165222719601	0.0074645901381386	0.8435156767394588	T	T	T
0.6100210974905502	0.1409782127711373	0.9433583722965263	T	T	T
0.6032467317769614	0.8359132625282523	0.9426722230287434	T	T	T
0.4186691640900821	0.8479580078866734	0.9725153721332075	T	T	T
0.4262817036027350	0.1544989555188265	0.9733457269287116	T	T	T
0.5335636094835133	0.9870258037828699	0.9911910642824239	T	T	T
0.4046754132811466	0.1538939856383204	0.8638510996296146	T	T	T
0.0684970454996642	0.8596912617825517	0.5846340574712643	T	T	T
0.0628390254149691	0.1659680938866978	0.5847316261887557	T	T	T
0.8860010377653151	0.8459010687176138	0.6149135411016203	T	T	T
0.8821901590365832	0.1540788324573273	0.6152882200673193	T	T	T
0.0734876097904490	0.8602194542255972	0.6383385605057649	T	T	T
0.9737385468030784	0.0029664753380897	0.6580741846381504	T	T	T
0.8719653111651658	0.1504960069139371	0.5581866896372407	T	T	T
0.8789852531057650	0.8453988237016692	0.5579177350086933	T	T	T
0.0660060649983063	0.8644114423953166	0.5290733347995077	T	T	T
0.0578786007307317	0.1709679398784943	0.5291950747124914	T	T	T
0.9524225246761716	0.0065129674193658	0.5102556844728455	T	T	T
0.0715581435582791	0.1518842642879415	0.6384683550750316	T	T	T
0.5680009315630344	0.8525582530769517	0.5843909677743614	T	T	T
0.5663074848189130	0.1590107136970887	0.5840497271317401	T	T	T
0.3852220883306827	0.8504334280388310	0.6145268020064129	T	T	T
0.3847094110610092	0.1587297891681206	0.6143934884357459	T	T	T
0.5731259923666946	0.8602331988873114	0.6380324628151387	T	T	T
0.4740484823143471	0.0067919082458593	0.6575308214139833	T	T	T
0.3762447846134758	0.1517924395034619	0.5572085339561764	T	T	T
0.3784310559396906	0.8464222949808686	0.5575217310163708	T	T	T
0.5655308274990301	0.8491354547085159	0.5287656439083079	T	T	T
0.5634741476216510	0.1560442857338183	0.5284847277699805	T	T	T
0.4551208623780416	0.9985902371677233	0.5096500550547896	T	T	T
0.5730687898692147	0.1520571028229609	0.6378426309400975	T	T	T
0.8221896227023713	0.8555382869889567	0.0846305712222384	T	T	T
0.8177963422214869	0.1618881143992308	0.0841987964761261	T	T	T
0.6406108762220043	0.8479191791061648	0.1152599105290460	T	T	T
0.6380514205085368	0.1561890042913912	0.1151581031600028	T	T	T
0.8289965860195672	0.8617620725627837	0.1382915032973188	T	T	T
0.7304462860096560	0.0077745302531727	0.1580083110065909	T	T	T
0.6264385457634929	0.1472500683086740	0.0579834041335243	T	T	T
0.6312131846479260	0.8420187191418192	0.0584681645434518	T	T	T
0.8169200353448158	0.8502717008450542	0.0291101117735510	T	T	T
0.8117535796920250	0.1570317096127966	0.0285632104768198	T	T	T

0.7039928455498498	0.9941086644063819	0.0102471365634305	T	T	T
0.8280797852811194	0.1536016208635157	0.1379618834535776	T	T	T
0.1646899220413437	0.8536621310033045	0.4172450149538385	T	T	T
0.1686457966371432	0.1600226401387318	0.4178357898487466	T	T	T
0.3465449707435730	0.8480602186563095	0.3867111826276813	T	T	T
0.3487187098303642	0.1563353908961091	0.3869770773886713	T	T	T
0.1581413811145750	0.8620128775746405	0.3636229447055979	T	T	T
0.2568652728289234	0.0083258873983795	0.3439901967094753	T	T	T
0.3597304637263247	0.1457011418112473	0.4441698726398023	T	T	T
0.3554194721820475	0.8404584357018784	0.4435419630392206	T	T	T
0.1695081544300825	0.8465908368832716	0.4728018090100894	T	T	T
0.1740436272056691	0.1533546592331751	0.4734827249568090	T	T	T
0.2819733735760463	0.9908382539456120	0.4917884259955933	T	T	T
0.1590670722179704	0.1538912356278362	0.3640270543652247	T	T	T
0.6636361798631308	0.8591832397280604	0.4169074599972212	T	T	T
0.6715171164440721	0.1652306721294791	0.4174484321824050	T	T	T
0.8458018142148197	0.8446518897209744	0.3864169634767085	T	T	T
0.8506674021646938	0.1528047587266617	0.3864335832381698	T	T	T
0.6580568515065370	0.8630384385626435	0.3632863812484027	T	T	T
0.7573527948653636	0.0072886175816320	0.3436096332718641	T	T	T
0.8627134583938277	0.1407485278099431	0.4437081799914595	T	T	T
0.8540608358018937	0.8358595132433194	0.4431286022569101	T	T	T
0.6676501641405589	0.8541235353080041	0.4722948326197339	T	T	T
0.6781417616044301	0.1603148261299709	0.4731863412865760	T	T	T
0.7828481290375675	0.9886117849757975	0.4913689270917645	T	T	T
0.6602883609384218	0.1547738779339557	0.3636391303745592	T	T	T
0.3202502301259294	0.8562128278860855	0.0843208558007219	T	T	T
0.3163150644535827	0.1626436245872465	0.0843251045006718	T	T	T
0.1400911765233435	0.8467622532641021	0.1154121295896585	T	T	T
0.1372712678066453	0.1549979907812082	0.1155772263575842	T	T	T
0.3293162493657028	0.8600618529638794	0.1380390406020327	T	T	T
0.2311596499946780	0.0040964859473636	0.1581083973927049	T	T	T
0.1238793877579422	0.1515949992863454	0.0586056588057751	T	T	T
0.1283668778484265	0.8463107289640346	0.0585338866679819	T	T	T
0.3126275744381268	0.8568286368944074	0.0286582531033078	T	T	T
0.3083405004720001	0.1636894652152967	0.0287975753185746	T	T	T
0.1993603781108436	0.0046287957042485	0.0104125682656023	T	T	T
0.3278788956782607	0.1519368811031919	0.1380330821476920	T	T	T
0.9702428391855932	0.0023025701720658	0.9167564168486517	T	T	T
0.0383905550339538	0.0017774371152784	0.8884264356658155	T	T	T
0.0477539926531397	0.9884153831327341	0.9436846923523226	T	T	T
0.9762148262109391	0.9886809906515910	0.9716801779533552	T	T	T
0.4713522933558189	0.0039230990379075	0.9167850196120026	T	T	T
0.5388590316217235	0.0018325967266278	0.8883582507452680	T	T	T

0.5494835937819328	0.9934515870673416	0.9436262876146141	T	T	T
0.4785612226867976	0.9958456879244024	0.9717267832101868	T	T	T
0.0087773019582186	0.0086114351880743	0.5849610983753050	T	T	T
0.9392830833354140	0.0028848774525551	0.6130723156169927	T	T	T
0.9326478139892799	0.0032462297366508	0.5577384734115998	T	T	T
0.0057817365079550	0.0116771830448688	0.5300265426066514	T	T	T
0.5102185905819704	0.0045458143057002	0.5844325893102077	T	T	T
0.4402036804101606	0.0048851956696508	0.6124792994947114	T	T	T
0.4345751519677110	0.0007410365551619	0.5571148478140705	T	T	T
0.5082480363646167	0.0011217637125078	0.5294685160446667	T	T	T
0.7631006547531043	0.0054818940941993	0.0848167786996672	T	T	T
0.6944601840299932	0.0038409501758024	0.1130696868301338	T	T	T
0.6860217735588594	0.9981851581383321	0.0577720467739800	T	T	T
0.7581603007153509	0.9999656543644277	0.0298764932132408	T	T	T
0.2235702357788129	0.0039404482345640	0.4171764475818613	T	T	T
0.2924801487565181	0.0036345437807307	0.3889578996017289	T	T	T
0.3003710772796790	0.9962673472929211	0.4442733680633852	T	T	T
0.2279746583856657	0.9967791333171022	0.4721300705901726	T	T	T
0.7244210641072939	0.0063866264503261	0.4167857562319303	T	T	T
0.7931218689221681	0.0022091048090387	0.3885471941099455	T	T	T
0.8012533615904729	0.9947508850937883	0.4438532465538456	T	T	T
0.7289766651716095	0.9996878544233959	0.4717245488606248	T	T	T
0.2614151084324763	0.0064986426119479	0.0848484034361593	T	T	T
0.1937382193540881	0.0029734788595630	0.1132436265625893	T	T	T
0.1833076674506590	0.0023413095429752	0.0579800482054593	T	T	T
0.2543446934651954	0.0070660357492503	0.0299072989719697	T	T	T
0.9569103785834298	0.0079512621376887	0.8629889457325048	T	T	T
0.4567796615731709	0.0066800197136923	0.8630372535632492	T	T	T
0.0195524901880504	0.0046856455518155	0.6387615012937312	T	T	T
0.5201101523054833	0.0060404936870502	0.6382524935965406	T	T	T
0.7755674538404662	0.0069583366545803	0.1385952772311411	T	T	T
0.2115829452999241	0.0072012580041186	0.3633811450866477	T	T	T
0.7121389123740607	0.0072321601310202	0.3630083898753439	T	T	T
0.2756473445146340	0.0049667123516980	0.1386068961712692	T	T	T
0.2598265703224327	0.0042050343654342	0.6852230707645967	T	T	T
0.2184917625677438	0.0045738608958139	0.8161167660802880	T	T	T
0.1905519150072580	0.5066427434570790	0.6226648829679240	T	T	T
0.2387132665527536	0.5048274696051760	0.7507900931770317	T	T	T
0.2876173178237462	0.5045493818826533	0.8789749414394393	T	T	T
0.9933011279523409	0.5030646416980787	0.6902831561643943	T	T	T
0.9845101655869507	0.5040753319968092	0.8112871118870276	T	T	T
0.7590946571256574	0.0029546355850117	0.6853194785667581	T	T	T
0.7187529196444558	0.0044524742862208	0.8160418141760517	T	T	T
0.6904903664963687	0.5037376725221323	0.6226545135578107	T	T	T

0.7388435195682101 0.5037730798733997 0.7508049660462658 T T T
0.7873251704645373 0.5042658263921871 0.8789967923254751 T T T
0.4933165767746953 0.5039861848213619 0.6902874451085713 T T T
0.4845573013981213 0.5045927086250133 0.8112775539059264 T T T
0.5143060706890371 0.0044746048341318 0.1854316466850412 T T T
0.4730734913489813 0.0048543038740265 0.3163336444287543 T T T
0.4449211008189775 0.5055786285956594 0.1226424987879103 T T T
0.4938098124102460 0.5050500266597218 0.2507978359199652 T T T
0.5419483615123918 0.5056703981945933 0.3789530689939520 T T T
0.2484173501040237 0.5040785342385090 0.1904273799450807 T T T
0.2391137137500895 0.5046439346096047 0.3114502170754602 T T T
0.0140199403113647 0.0038417812515408 0.1855457864818551 T T T
0.9731709917845971 0.0044172139259335 0.3162254200511012 T T T
0.9454381363778460 0.5048192124534001 0.1227447065828802 T T T
0.9937278879616176 0.5041877102480906 0.2509020096013752 T T T
0.0415349707044872 0.5044131663793234 0.3790637005866521 T T T
0.7484182600761353 0.5044066885689483 0.1903687304011490 T T T
0.7391402060488863 0.5047443300469900 0.3113735590720165 T T T
0.2382411403426320 0.5041257844614097 0.6854904198389480 T T T
0.2398102508440910 0.5047905656726107 0.8160148107250480 T T T
0.7380315254246117 0.5031005079820874 0.6855633731342651 T T T
0.7397813817590093 0.5044863823481803 0.8160634459816375 T T T
0.4931780289412861 0.5042522735590118 0.1855736151469970 T T T
0.4941866733521363 0.5047515612532267 0.3160488394948660 T T T
0.9932456512009649 0.5036985115904679 0.1856746014848297 T T T
0.9941526374487978 0.5041822987754215 0.3160694949344280 T T T
0.9886402089127857 0.0038978684772517 0.7508088497843837 T T T
0.4888681235058132 0.0034001864865081 0.7507180115197221 T T T
0.2437602683646978 0.0047190127717413 0.2509769948102545 T T T
0.7437625148490782 0.0040200640070842 0.2507807615840293 T T T

(17)PR_2SnBr_4 (D-J-1)

D-J-1-PR2SnBr4

1.00000000000000

5.7609224276094739 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.7375811063451581 0.0000000000000000

0.0000000000000000 0.0000000000000000 16.2385406494140625

H C N Br Sn

22 8 2 4 1

Selective dynamics

Direct

0.8281111294344728 0.9005031757607952 0.3095366066795543 T T T
0.8291543790339078 0.2092201248740636 0.3099109525740669 T T T
0.1996180294022292 0.8995974243674731 0.2269067866383307 T T T

0.1998686291598320	0.2097069085270016	0.2270695202725618	T	T	T
0.8270082215959492	0.9078222164393885	0.1568251637678865	T	T	T
0.2081107058230978	0.2068055243737687	0.3875808550253774	T	T	T
0.2075860605702668	0.8992064240911374	0.3870854755357162	T	T	T
0.8312515292950234	0.8987525174651222	0.4662730018430113	T	T	T
0.0323444288140545	0.0553213267039457	0.1038324939613107	T	T	T
0.2208665402392471	0.8999926270300077	0.6996595296606306	T	T	T
0.2201112017504492	0.2086550650461295	0.6992813285506012	T	T	T
0.8619485368323953	0.8987105420707694	0.7885694910424872	T	T	T
0.8614759317786643	0.2100599954089304	0.7882625003476549	T	T	T
0.0594748957347050	0.0557940361365723	0.9083942500076116	T	T	T
0.8350054845739220	0.2067456446730208	0.6256899125497746	T	T	T
0.8353802574144024	0.8989039733804693	0.6261389665568813	T	T	T
0.2081896951244427	0.8983981024512404	0.5449077150242492	T	T	T
0.2459416074869638	0.2037460962678556	0.8492940306958460	T	T	T
0.8309777204572824	0.2060633375348070	0.4665216682381615	T	T	T
0.2090030169577065	0.2055100397387850	0.5447881201685542	T	T	T
0.8271788262157155	0.2026512449535334	0.1569702089792097	T	T	T
0.2461679856033229	0.9070229926937579	0.8496049349916636	T	T	T
0.9428235438700636	0.0544640797680618	0.3098852131823271	T	T	T
0.0881257572294508	0.0547257070301116	0.2315644173468740	T	T	T
0.0925496518942042	0.0532080132599377	0.3876426857174519	T	T	T
0.9466319480136669	0.0525056512355173	0.4664929057513989	T	T	T
0.1061530041478290	0.0540626915451530	0.7008634847701269	T	T	T
0.9715922707059729	0.0544905259497860	0.7816068956013812	T	T	T
0.9502454829597066	0.0529584389094237	0.6246586067339860	T	T	T
0.0928929694652759	0.0522550575498523	0.5450389494558801	T	T	T
0.9336912257089556	0.0551563319299482	0.1571289684935283	T	T	T
0.1402161985809372	0.0553098542449352	0.8518804935077244	T	T	T
0.4393322687887571	0.0550418686366625	0.0301892159755377	T	T	T
0.4615143499709946	0.5550026124003837	0.8237587349103865	T	T	T
0.9750180883718856	0.5547437047096250	0.9880672652893766	T	T	T
0.6041961296048272	0.5548962239594786	0.1913275778174445	T	T	T
0.4954732973894305	0.5550538988825652	0.0112370723354491	T	T	T

(18)$PR_2CsSn_2Br_7$ (D-J-2)

D-J-2-PR2CsSn2Br7

1.00000000000000

5.8313747315103841	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.8232682854836755	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.6754398345947266

H	C	N	Br	Sn	Cs
22	8	2	7	2	1

Selective dynamics

Direct

0.8487314392425019	0.8982974050151581	0.3586360164980618	T	T	T
0.8520547635988763	0.2022455759107796	0.3584481405142064	T	T	T
0.2209628710333286	0.8933481643212418	0.2988462834025842	T	T	T
0.2228662726969463	0.1990207437823319	0.2983782631047939	T	T	T
0.8564039693893939	0.9024365436943489	0.2446285034068895	T	T	T
0.2200916507880949	0.1984318671573141	0.4195977506234276	T	T	T
0.2172750416936564	0.8953921622337457	0.4196513450358638	T	T	T
0.8375667167443139	0.8988368451747304	0.4752582033951707	T	T	T
0.0607032574653231	0.0455832142596754	0.2053949859382826	T	T	T
0.1918480490122146	0.8978356451819797	0.6546393781814178	T	T	T
0.1881662034285465	0.2017718612552905	0.6550352676626128	T	T	T
0.8203945288839317	0.8918293997247971	0.7147354899559150	T	T	T
0.8177130711861126	0.1974966694819455	0.7152790937026378	T	T	T
0.9811604401899918	0.0444032183225940	0.8080825679021237	T	T	T
0.8200718760706803	0.1984328298294764	0.5940207421908259	T	T	T
0.8226225442620293	0.8953981495373673	0.5937968262263670	T	T	T
0.2022330408850354	0.8987451045422062	0.5382142546028635	T	T	T
0.1837555650103205	0.1906278126638107	0.7690961953147579	T	T	T
0.8392249019250951	0.2013862485662941	0.4749970562087499	T	T	T
0.2008114293059313	0.2012946305195815	0.5384715421436347	T	T	T
0.8574561037653217	0.1914284255511080	0.2442840677027794	T	T	T
0.1854108156866028	0.9016725717612348	0.7686908667105045	T	T	T
0.9633427715197934	0.0490519893921349	0.3594119140625672	T	T	T
0.1115939785464415	0.0469378911588843	0.3016011272295009	T	T	T
0.1048423580033268	0.0479700339591173	0.4188442963842323	T	T	T
0.9526109681235835	0.0495044913411079	0.4764669052922315	T	T	T
0.0770585544420932	0.0484593722489635	0.6540248215616831	T	T	T
0.9293366368712023	0.0457134274115804	0.7119269298832610	T	T	T
0.9351931685309681	0.0478684578918483	0.5946503985756842	T	T	T
0.0873024514811538	0.0494969803148615	0.5370048981508392	T	T	T
0.9621605073991429	0.0466219851651863	0.2450954338133843	T	T	T
0.0793702881936664	0.0456335688084764	0.7683186799785426	T	T	T
0.5644744897020700	0.0471509385436469	0.8668446876607644	T	T	T
0.4262580673160126	0.5480750537694109	0.7354144885576448	T	T	T
0.5218758101497476	0.5482779162092307	0.0063653482001435	T	T	T
0.0331121653407694	0.5470678714854220	0.8782181401653101	T	T	T
0.4785003679116898	0.0483053795811096	0.1461008878941147	T	T	T
0.6156621357656383	0.5485331968645691	0.2774446465793271	T	T	T
0.0100607571431043	0.5485088604388288	0.1345941218304871	T	T	T
0.5201386173139744	0.5471014831625209	0.8681399181023955	T	T	T
0.5231525614598095	0.5486051314533188	0.1445629911171705	T	T	T
0.0216647925215732	0.0482608823127816	0.0065365245362528	T	T	T

(19)$PR_2Cs_2Sn_3Br_{10}$ (D-J-3)

D-J-3-PR2Cs2Sn3Br10

1.00000000000000

5.8284430549931949	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.8217387370464619	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.4098606109619141

H	C	N	Br	Sn	Cs
22	8	2	10	3	2

Selective dynamics

Direct

0.8491356886290552	0.8851202220461419	0.3600017530768784	T	T	T
0.8416153975724879	0.1890645521432680	0.3595681509712065	T	T	T
0.2148736268989085	0.8908866420405203	0.3109095675732674	T	T	T
0.2095889909467535	0.1965768748119366	0.3106945229969355	T	T	T
0.8443950453779001	0.8929844294415734	0.2697975279215595	T	T	T
0.2143292207618797	0.1995038849379763	0.4062395566648548	T	T	T
0.2223022072135445	0.8964611944544073	0.4066584102071133	T	T	T
0.8452386500402894	0.8882960383853716	0.4518674758455908	T	T	T
0.0444254112686553	0.0377100473038240	0.2378307149268789	T	T	T
0.1978698207885546	0.8942326061845729	0.5932104570647008	T	T	T
0.1971735997756512	0.1983103051681629	0.5931399308310308	T	T	T
0.8253075842014875	0.8932714828692054	0.6404503196925903	T	T	T
0.8262745548426103	0.1990363142135406	0.6406177371659763	T	T	T
0.9862192134752891	0.0454508796137783	0.7142823046342394	T	T	T
0.8269044897197682	0.1957147646736261	0.5451880994831378	T	T	T
0.8298177490368883	0.8926342797349622	0.5450820010525242	T	T	T
0.2106049590570498	0.8981344907697207	0.5009338971333442	T	T	T
0.1912207663402759	0.1886984042398888	0.6834714180691791	T	T	T
0.8376663795166504	0.1907922723618199	0.4515177427224306	T	T	T
0.2041390722543997	0.2007476897991926	0.5004697666025444	T	T	T
0.8420192319196779	0.1818333327238514	0.2691960756040664	T	T	T
0.1897285134199968	0.8999329951527092	0.6834868433779001	T	T	T
0.9583829914707462	0.0398846324281917	0.3599593664672670	T	T	T
0.1021175277018442	0.0418566085425172	0.3136262852261287	T	T	T
0.1044541935492667	0.0449818323725811	0.4063097906451650	T	T	T
0.9557764730049998	0.0424298544189865	0.4523852660526363	T	T	T
0.0845457012297350	0.0460135548585337	0.5925174639846488	T	T	T
0.9361516355550081	0.0458383626297678	0.6382032974465640	T	T	T
0.9422975312431630	0.0452618610571706	0.5456394381900738	T	T	T
0.0931474743217186	0.0469727054945514	0.4998805704165172	T	T	T
0.9484323639885592	0.0383649834858085	0.2696020435609779	T	T	T
0.0852386594814448	0.0448474145471009	0.6829266803304129	T	T	T
0.5716227834887816	0.0421724241063101	0.7597137772913088	T	T	T
0.5119557345191021	0.0403305972757971	0.9764428315533018	T	T	T

0.4332528084460222	0.5442506652025053	0.6557030232956927	T	T	T
0.5202974570944807	0.5417508698834909	0.8694990755461836	T	T	T
0.0380292740636474	0.5416445656721911	0.7688110070374442	T	T	T
0.0111353250541372	0.5405292985002245	0.9764403644231129	T	T	T
0.4594378489084792	0.0391081928196763	0.1927955707841747	T	T	T
0.5040450232772800	0.5401437251647465	0.0835925845694216	T	T	T
0.6007759755168797	0.5403402048232306	0.2973750842080096	T	T	T
0.9893282647691535	0.5390806150925572	0.1836687301011037	T	T	T
0.5253564783012056	0.5419161287953028	0.7600516223563366	T	T	T
0.5111655662457598	0.5397744558530538	0.9765206198715987	T	T	T
0.5029535275365818	0.5389067247385750	0.1930035980163559	T	T	T
0.0215791001377505	0.0411075480272643	0.8724827229954397	T	T	T
0.0029001080364908	0.0401584711398483	0.0803189120121734	T	T	T

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