

Supporting Information

Ga and In-based hybrid halide perovskites as an alternative to Pb: A first principles study

Tridip Chutia^{1,4}, Tanmoy Kalita², Uddipana Saikia³ and Dhruba Jyoti Kalita¹,

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^{1, 2, 3}Department of Chemistry, Gauhati University

⁴Department of Chemistry, Bhattadev University, Pathsala, Bajali-781325, India.

Electronic mail: dhrubajyoti.kalita@gauhati.ac.in

Table S1: Optimized coordinates (X Y Z) of the studied compounds (in Angstroms):

(MA)₃ (Ga_{.25} In_{.75})₂ I₉

Ga	1.1207047063	0.7225721577	0.5741959219
Ga	1.1601235704	5.8991942225	6.8513562670
In	6.1786332122	12.3712608489	6.9419889732
In	12.5788278817	12.5560457586	11.9162486684
In	7.5750386461	1.0701276845	5.3517465753
In	7.4672219894	5.8047937277	11.7904767085
In	12.3363853773	7.3641672376	5.7894446455
In	6.0850321689	7.4438693899	0.5067316464
H	4.1159187393	10.5850522877	2.7602066786
H	2.9046422129	9.3257656993	2.3342299258
H	10.4406025064	9.3185121853	2.9970429628
H	10.7397851460	3.5129674252	7.9901581271
H	9.3071947817	4.6016267186	3.5924422814
H	9.0124443250	3.2578639128	2.4295691009
H	10.1742130712	10.6135022155	1.7821572006
H	4.2859419092	1.9814683169	9.3396581107
H	8.9283556904	10.3969084147	10.5839825768
H	7.9924746451	9.2041114721	9.6106911684
H	4.5399665760	3.7464320378	9.5676799862
H	4.8518263591	4.5283177525	2.6657988238
H	10.6352553283	4.5230684617	9.4801365045
H	4.0772282153	10.6942129720	10.3024402721
H	4.0481821442	9.0361837085	3.6774450979
H	10.6348042879	11.0385015134	3.4638685555
H	3.3193388956	3.1663599964	8.3820290039
H	9.1474809719	4.1446683038	8.5421184682

H	9.8337784280	4.7653055201	1.8821803951
H	4.5830610663	2.8408643309	2.1133779101
H	3.1710367800	10.2876689958	8.8205332195
H	4.6484478835	9.3708592442	9.2413739341
H	9.3706701956	8.6469923571	10.6219097738
H	3.2334958727	4.0338669058	2.0680089973
H	9.3694209166	2.7355828722	10.5537464047
H	2.0449352407	9.3408864179	10.7301971740
H	9.9255618653	8.8253504492	8.2188028384
H	1.9865373189	2.2977321837	10.1875762454
H	4.5973027990	3.0995032012	4.5724397010
H	11.6692773722	4.2400894162	3.3885904758
H	3.2756109735	4.1032847853	4.5027129102
H	10.9440091840	2.7736456833	3.8342549104
H	9.6224553148	10.4666313318	8.2666744130
H	8.0834901955	9.6245847994	2.7942923858
H	2.2951310379	3.9135010852	10.4722165142
H	3.4090783603	8.5414893977	11.2563156170
H	8.4738131647	10.3053807386	4.2403077565
C	3.8029600450	2.9664663812	9.3462526477
C	9.6948393227	4.0674986238	2.7168641236
H	1.8752180644	11.1275207400	3.6548908667
C	8.9791113623	9.4676337744	10.0060393598
H	1.8645740740	9.7294770407	4.5675900029
H	3.1286316769	2.7066941952	11.3338848699
C	3.4591830238	9.7996249429	3.1537943348
H	10.8800664865	9.8327943657	9.1827446124
C	3.7686759112	9.8831162639	9.6402618191
C	4.1292973113	3.7085112531	2.6076305065
C	10.0725338537	10.3365606460	2.8377654002
H	2.9677434411	10.9359022043	4.8882239326
H	10.8460095451	2.1224096042	9.9728905296
C	10.1279632842	3.7709710764	8.8629722012
H	11.4936605073	3.0438633286	2.2513058663
H	9.4179440523	1.8010123932	9.1806576330
H	2.6643778328	8.0828326329	9.8556441722
H	3.0973787704	2.5209643473	4.0111280523
H	8.1858578732	11.3054406843	2.9198183245
N	2.9447618911	8.9185182588	10.4056968887
N	3.7460415522	3.3243265268	3.9985553902
N	8.6309136893	10.4030917722	3.2163478180
N	2.7505618982	2.9762312413	10.4058830583
N	9.9084945635	9.6654240192	8.8491347946
N	11.0287748596	3.4851753336	3.0696540466
N	9.9303804213	2.5398701386	9.6944310616
N	2.4930878278	10.4149815656	4.1116681332
I	9.9246226460	13.0998644486	12.5674504981
I	7.1653664082	0.6052837081	2.6046964028
I	13.0726872508	13.7971590491	9.3896168743
I	6.9106526919	12.8834659474	9.5782978058
I	3.5519125966	6.5497879512	6.0293394042
I	9.7222367141	6.8053132827	6.5857381416

I	6.4766330534	6.3647609778	9.2154813359
I	7.1153759605	3.0448466624	12.0852529425
I	12.6363085365	10.1487735548	6.3025631133
I	6.3771460463	10.1881229099	0.0516095910
I	1.0545000157	5.9794874442	9.5278760451
I	12.4989955426	6.9629138372	3.0084326544
I	3.2775687847	6.9500372120	0.3326507390
I	10.3655226661	1.0620502021	5.7556785601
I	6.9174551222	7.1515824724	3.1810259487
I	12.6670530192	9.7969624007	11.2868461147
I	6.7255741772	3.6828506607	5.8374593814
I	0.7806251902	0.3352260885	3.1694209941
I	3.6561614537	0.4932939097	-0.0000397402
I	10.2500185115	6.1726926743	12.0964539771
I	0.4848409960	3.2999244083	0.3414538338
I	0.7448864536	3.3830530058	6.1441943344
I	3.3855561907	12.6672763436	6.7294505649
I	6.7919295039	9.7051023570	6.3912272087

(MA)₃(Ga_{.50}In_{.50})₂I₉

In	0.9517276001	0.5267131924	0.6086413992
In	0.9160416408	6.0779464757	6.7131343632
Ga	5.9162236422	12.3521723795	6.9056057477
Ga	12.4867752846	12.5226573860	11.7981303194
In	7.4643600121	0.9365303987	5.5965648385
In	7.4395382862	5.8934818633	11.8876488442
Ga	12.3212004507	7.7978823883	5.6264876545
Ga	6.0920515436	7.3029506688	0.5923507946
H	4.0176428780	10.8852813328	2.7281389841
H	2.9750964581	9.5340916295	2.1696891611
H	10.5237028352	9.4193875748	2.5820270300
H	10.9406110814	3.7834177110	8.1934817224
H	9.3016269579	4.4320308293	3.6663464345
H	9.0459931640	3.5834594279	2.1090089195
H	10.0752948158	10.9549671949	1.7478505000
H	4.3120710995	2.0309235384	9.5717083252
H	8.7024335530	10.4657530211	10.4053753952
H	8.0883485706	9.2085972878	9.2702387762
H	4.3929330597	3.8233069599	9.4381742568
H	5.1156647430	4.0768671894	2.6320387981
H	10.3568360233	4.5995589191	9.6986414606
H	4.1493596423	10.6455008369	10.1299160126
H	4.2898722109	9.2176573547	3.3331563551
H	10.6488145308	10.9856666849	3.4539170978
H	3.1705168821	2.9073775110	8.4868723672
H	9.1991711247	4.1931454447	8.3810280497
H	10.2821277945	4.8819972342	2.2215216128
H	4.3661413772	2.4668859544	2.3562040749
H	3.1440864840	10.0709700751	8.7693395626
H	4.6575448520	9.2162590738	9.1914185462
H	9.4126716314	8.8150752072	10.4190749114

H	3.3919206750	3.9626754292	2.1593158952
H	9.1213527134	2.5675735094	10.2559270977
H	2.1853518833	9.3342585053	10.8671711047
H	10.0726665808	9.3123464189	8.0126194900
H	1.9938585461	2.3633769234	10.4821214188
H	4.5974096239	3.1321442544	4.7754116186
H	11.4107897740	3.3277300113	3.9364419587
H	3.5520962865	4.3877768131	4.5301332478
H	10.3977824228	2.1244234892	3.3583393796
H	9.7415500826	10.9164324675	8.3298406627
H	8.0952889246	9.7060365445	2.5172111882
H	2.2541008160	4.0148886152	10.4834960620
H	3.6009397845	8.5646077226	11.3376706407
H	8.5920860825	9.8387193817	4.1098998663
C	3.7295546229	2.9500812228	9.4295286674
C	9.7891683761	4.0613160114	2.7576514018
H	1.8017848299	10.8042186303	3.8502434688
C	8.9693862301	9.5976798692	9.7938545174
H	2.2063242643	9.3168152901	4.5141661222
H	3.1755417475	2.9983594023	11.4771720597
C	3.5381468767	9.9438227976	3.0128736146
H	10.9282716168	10.1284430880	9.2122464895
C	3.8013013847	9.7629519367	9.5889019334
C	4.1978426257	3.4839895135	2.7268221914
C	10.0821012580	10.4168532579	2.7058685677
H	3.0587637756	10.6967512714	4.9295980557
H	10.7455521889	2.1846299743	9.9728774803
C	10.1101058158	3.8800405521	8.9054889404
H	11.4923296175	2.8955419053	2.3231928614
H	9.6221232530	1.8395822496	8.8005013630
H	2.7301608230	7.9993574734	10.0448411916
H	2.9890938371	2.8257102703	4.3404199910
H	8.2154494026	11.2237546736	3.2135864372
N	3.0498200221	8.8728850694	10.5118238698
N	3.8035659822	3.4374301136	4.1664703896
N	8.6664127370	10.2776048390	3.1740791286
N	2.7409817613	3.0908016721	10.5440132307
N	9.9871714910	10.0181186539	8.7789962100
N	10.8275039548	3.0379392491	3.1228579286
N	9.8755533475	2.5410495718	9.5297651256
N	2.5999525418	10.1952471709	4.1407509336
I	9.9497632100	12.9537953553	12.2059082089
I	7.7000449736	0.6486799673	2.7736873844
I	13.1490929218	13.8233197188	9.5609467652
I	6.5869458160	12.7465434979	9.4080122868
I	3.5495400814	6.5851347896	5.8565646030
I	9.7715917087	7.4466238010	6.1206798980
I	6.4517198426	6.4695921097	9.3190431090
I	7.1878193443	3.0772473051	12.0416814182
I	12.9037092243	10.2218743106	6.4931861142
I	6.3763633514	9.9217303207	0.2024929601
I	0.9648132370	6.0410014909	9.5747263661

I	12.8242948766	7.6280244623	3.0612581412
I	3.4604937951	6.8274001633	0.3897398306
I	10.1494350470	0.5907887372	6.4537513487
I	6.8076096117	6.9198890970	3.0861856051
I	12.7439057938	9.9558997808	11.2234471796
I	6.8546466150	3.6429135782	6.0274390504
I	0.4375747073	-0.0880199077	3.3002715761
I	3.6796273007	0.4180692144	0.0394674314
I	10.2068313024	6.3425128772	12.1430427478
I	0.3138283952	3.3037299638	0.5391502462
I	0.4440193875	3.3974850007	5.8497511792
I	3.3438002704	12.8302358750	6.6232450117
I	6.2823003763	9.8405689305	6.2416604207

(MA)₃(Ga_{.75}In_{.25})₂I₉

Ga	1.1225026776	0.7562584468	0.5079360145
Ga	1.0470719858	5.8312302508	6.7341046652
Ga	6.3277968410	12.4682550373	6.8591475427
Ga	12.5582823870	12.8029241545	12.0051298433
Ga	7.5416112649	0.9034549164	5.3591786964
Ga	7.4794418808	5.7531872856	11.8163275346
In	12.4773776107	7.5616575851	5.6311027027
In	6.2168111811	7.2627435327	0.4979717745
H	4.1427350555	10.4463814660	2.6375377849
H	2.7615266372	9.3153477517	2.4791340764
H	10.5797283155	9.6269373769	2.4223078089
H	10.6612827271	3.2706864687	7.9563018924
H	9.5069463310	4.4765010694	3.7794229941
H	8.8239169993	3.4838318180	2.4581664146
H	9.9761740436	11.2456186783	1.9149775521
H	4.2783235611	1.9189226177	9.7557862539
H	8.9715698889	10.3285433182	10.6501459218
H	8.0323288328	9.3184559242	9.4998412610
H	4.5425870668	3.6801065207	9.5343990945
H	4.8044719475	4.4674227465	2.7595304945
H	10.6647551907	4.3786558357	9.3744385292
H	4.1493255397	10.6437069771	10.3823559542
H	4.0264562026	9.0139351820	3.7080973279
H	10.5886377431	10.9935523428	3.5795769540
H	3.3497205646	2.8111428697	8.5097858149
H	9.1699905337	4.1621790961	8.4157635551
H	9.9822303487	4.7956128275	2.0781512706
H	4.5957782226	2.8090189615	2.1043048321
H	3.2565404405	10.3512224587	8.8505094470
H	4.6265873366	9.2784615483	9.3117279569
H	9.4430774021	8.6206314959	10.3628329582
H	3.1904715024	3.9261511829	2.1831915045
H	9.1949488473	2.8584122963	10.5420145241
H	1.9989409522	9.4948115276	10.7559375239
H	9.9501035164	9.2421960248	8.0271632738
H	1.9587232727	2.4493361475	10.4314071678

H	4.6787661063	2.8742303912	4.5539014517
H	11.7126117921	3.5237468984	3.2267313537
H	3.3699568941	3.8919591798	4.6135426438
H	10.6358887059	2.3212680622	3.6634755607
H	9.5698445647	10.8425792323	8.3769769073
H	8.1177708410	9.7960854228	2.3794090907
H	2.2845795720	4.0836381887	10.3185268078
H	3.2685648289	8.5130053105	11.2477857656
H	8.6644390706	9.4553099184	3.9366134377
C	3.8044979809	2.8718464051	9.5031655394
C	9.7092582884	4.0243808247	2.8046171864
H	2.1083704771	11.3337082113	3.6940068421
C	9.0257845848	9.5257244988	9.9089482349
H	2.0040930179	10.0295271603	4.7174751668
H	3.0723958735	3.1285194994	11.4666586653
C	3.4592825920	9.7855393085	3.1785160295
H	10.8876716458	10.1214226778	9.1291890553
C	3.7889241355	9.8793948656	9.6848142869
C	4.1200368708	3.6163413523	2.6707003688
C	10.0540978323	10.5325283498	2.7430782377
H	3.2795887124	11.0894791550	4.8553459889
H	10.5307297823	2.0014893138	9.9677649873
C	10.0724485854	3.6688469502	8.7885539799
H	11.0403396345	2.5718503489	2.0448387765
H	9.0385554001	1.8624840638	9.2228495340
H	2.4796241421	8.2093744382	9.8179297298
H	3.1575797350	2.3238238206	4.0435661323
H	8.1565828392	11.0064583761	3.5055968847
N	2.8424628901	8.9845653813	10.4114981802
N	3.8031411979	3.1318215031	4.0465521071
N	8.6763315562	10.1660667101	3.1824510496
N	2.7278891622	3.1526244292	10.4939285026
N	9.9173088870	9.9610104789	8.7902674013
N	10.8394752776	3.0525158750	2.9397174889
N	9.6854678324	2.5380613603	9.6802254574
N	2.6816688086	10.5912065734	4.1617716143
I	10.1280687960	13.4540656357	12.7488959790
I	7.0358126110	0.4107271405	2.8248720266
I	12.9751867036	13.9535770438	9.6304056520
I	7.2288298640	12.8558669183	9.3273366175
I	3.5269279847	6.2548140122	6.0298114304
I	9.7306768860	7.3872592676	6.1717209785
I	6.6303733507	6.2362933065	9.3825910145
I	7.0457701063	3.1784826717	12.2534784316
I	13.0672520718	10.1904395288	6.5575355888
I	6.6967196704	10.0450475847	0.1805588929
I	0.9263898675	6.0478872778	9.3958999266
I	12.7601871357	7.5184889603	2.8511341983
I	3.3841070314	6.9633468977	0.2165774925
I	10.1690109311	0.6877584001	5.6542890595
I	6.7771112736	6.8575919869	3.2134149643
I	12.5988200104	10.2138260113	11.4379467346

I	6.9147044261	3.3948111302	5.8489593913
I	0.7263845818	0.3181422091	3.0939024620
I	3.6148837199	0.3346929671	-0.1119682275
I	10.0912051857	6.0606086125	12.0245312579
I	0.6447212650	3.3696341485	0.4043208341
I	0.4957670041	3.3432627745	6.0614543284
I	3.7268389013	12.9999482923	6.7251563548
I	6.4768556533	9.9010179460	6.3737382471

(MA)₃Ga₂I₉

Ga	1.0531780087	0.6661391631	0.4521001994
Ga	0.8969901656	5.9849290697	6.5874971379
Ga	6.2441460509	12.4821814939	6.8669048431
Ga	12.4948017303	12.8172183592	11.8919641748
Ga	7.4804116552	0.8696093764	5.3211522443
Ga	7.3128531575	5.8607370212	11.8544268849
Ga	12.5167881230	7.6910823034	5.5610157489
Ga	6.1871010746	7.3258593353	0.4073218568
H	4.1543122283	10.5533549240	2.6046970694
H	2.8770994496	9.3067768135	2.3933494910
H	10.5983522023	9.6200129326	2.3577034124
H	10.4935279378	3.1716470866	7.9430716600
H	9.4718712486	4.4267828727	3.7415919459
H	9.0278540978	3.4261155859	2.3274278173
H	9.7321852058	11.1226810424	1.8593258398
H	4.3200683420	2.0087788354	9.7197077413
H	8.9775160481	10.4299788490	10.6203611968
H	8.0526906936	9.4158355784	9.4555672732
H	4.4747470617	3.6831850300	9.0871223819
H	4.9121728694	4.2920603061	2.7783759456
H	10.6536689673	4.3699862201	9.2770591002
H	4.0062728178	10.6889809521	10.3389385631
H	4.1676431305	9.0600759541	3.6093615155
H	10.5703390352	11.0478872724	3.4453583346
H	3.0442622979	2.6785662431	8.6461417787
H	9.0844901550	4.1824069908	8.4265721258
H	10.1904089590	4.7769606960	2.1304311367
H	4.5082845058	2.6424383797	2.1783968404
H	3.1603249831	10.2579836765	8.8155796467
H	4.6056099434	9.3282831301	9.3303082337
H	9.4167390654	8.6963690650	10.3877647165
H	3.2484398982	3.9298206102	2.1967980318
H	9.1931349323	3.0337681832	10.6327883821
H	2.0023647863	9.4123264385	10.8108351742
H	10.0133655449	9.2615217449	8.0553005750
H	2.4125434430	2.7212606811	11.0246028361
H	4.5860999081	2.8017153087	4.6206499823
H	11.6945953529	3.5149314919	3.6924214315
H	3.3799799229	3.9531725124	4.6193079368
H	10.6386892957	2.2318246369	3.6592863336
H	9.7064073393	10.8762948214	8.3752024249

H	8.2021786886	9.3762251051	2.6920067292
H	2.4411630014	4.2529369127	10.3518073883
H	3.3248685518	8.4568403642	11.2241402288
H	8.9715423008	9.3827280039	4.1771624758
C	3.7750639317	2.9127099004	9.4277224445
C	9.8335084068	3.9923303021	2.8052081067
H	2.0761278523	11.2140097633	3.6910848491
C	9.0349526151	9.6024861096	9.9032408966
H	2.0575815793	9.8424190813	4.6337205428
H	3.7003477417	3.7283674793	11.3604723831
C	3.5369228489	9.8036709654	3.1120401092
H	10.9512567461	10.1003218334	9.1931126388
C	3.7173603223	9.8690090718	9.6733832407
C	4.1312497366	3.5254967900	2.7049175528
C	10.0068273779	10.4756616081	2.7001224088
H	3.2464717813	10.9909048730	4.8562016838
H	10.4236367080	2.0509539480	10.0322553729
C	9.9825767390	3.6639001209	8.7770829538
H	11.4268930508	2.7273635775	2.2426742756
H	8.8746146756	1.9623117735	9.3933982826
H	2.4745641257	8.1610167361	9.8241270657
H	3.0269825837	2.3859511352	4.1062734175
H	8.1460686996	10.7545528264	3.6290523775
N	2.8422107622	8.9288912983	10.4221568737
N	3.7473414773	3.1279344426	4.0938181902
N	8.7591494807	9.9685569714	3.3418898079
N	3.0407387188	3.4368856446	10.6167616687
N	9.9865834491	9.9839693847	8.8118252352
N	10.9616284440	3.0605928147	3.1080049312
N	9.5910009447	2.6209780331	9.7671077493
N	2.6930351205	10.4894113386	4.1292713837
I	10.0373184194	13.3367890189	12.6268301957
I	6.9344568695	0.2976354709	2.8186270798
I	12.8732719232	14.0098949051	9.5675633047
I	7.0911732467	12.9599134194	9.3391600850
I	3.4085222911	6.3287032996	5.9063778324
I	9.9104424393	7.4903126232	6.0182102452
I	6.5260032227	6.3662173923	9.3932129283
I	6.7076969966	3.3192447896	12.3176989389
I	13.1364273637	10.0602246289	6.5907206925
I	6.5365396272	9.9133150833	0.1138261135
I	0.8433854472	6.0430925815	9.2719069003
I	12.9434117674	7.7413415767	2.9874804085
I	3.5604633774	6.8350037769	0.1434323979
I	10.0944081195	0.5359033339	5.6168807719
I	6.7603092568	6.8686295447	2.9383831436
I	12.6182266868	10.1933861939	11.3976629518
I	6.9801751421	3.4170847019	5.7658717715
I	0.6555232792	0.1415909511	3.0298982599
I	3.5361140543	0.2026339183	-0.1543866717
I	9.9400074167	5.9787906122	11.9723390326
I	0.6188166884	3.3032867607	0.4069285368

I	0.2879015533	3.5010888501	5.8850073389
I	3.6378660232	12.9730396089	6.6831156049
I	6.4521686915	9.8994667611	6.4006819078

(MA)₃In₂I₉

In	1.1016948193	0.5960266335	0.6543753344
In	1.1332899986	6.0182676250	6.9521654518
In	6.0246070534	12.3510967760	6.9503053551
In	12.4786602427	12.4503957612	11.8544990999
In	7.4717116280	1.1529009419	5.4694752451
In	7.4746266880	5.7923138235	11.7898325769
In	12.2202989740	7.5636416095	5.7768977914
In	6.1086796146	7.3054153417	0.6185317744
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H	2.9865980846	9.4968697724	2.1862339349
H	10.4415993040	9.4630122240	2.7511024574
H	10.9932949704	3.7414509369	8.1127523451
H	9.3702824579	4.6100573436	3.6462747694
H	8.8954841713	3.4390840020	2.3750327049
H	10.1766109188	10.9118839892	1.7207880201
H	4.2893316892	1.9754210629	9.3099317998
H	8.8400382508	10.4189745179	10.5156081553
H	7.8730846431	9.1657107493	9.6655608171
H	4.5278419662	3.7339665108	9.5323682816
H	5.0429263440	4.4129857290	2.4668426321
H	10.5558821807	4.5755915726	9.6501560493
H	4.6776349154	10.2061032137	9.8452236989
H	4.3257547682	9.3037111009	3.3708466281
H	10.6476982602	11.1061925457	3.4347828417
H	3.2421397751	3.1408662979	8.4372616323
H	9.2964726422	4.2151239967	8.4292136921
H	9.9535536328	4.8392606860	1.9639441892
H	4.5963553152	2.6920980030	2.2272839351
H	3.1271684636	10.3315734708	8.9484893303
H	4.0695625196	8.7998631780	8.9135504195
H	9.2921939732	8.6873401340	10.6515345660
H	3.3719824270	3.9785654663	1.9799101759
H	9.2594260594	2.6229771315	10.2952535828
H	2.6734765868	9.9566986972	11.2819564326
H	9.7370242249	8.7012710350	8.2242294907
H	2.0357670825	2.2488841996	10.2598167609
H	4.6841287999	3.3550905050	4.6021635121
H	11.6700758286	3.8996145976	3.3811269662
H	3.4960858646	4.4828218450	4.3637897940
H	10.7167757906	2.5788572449	3.7992265917
H	9.4042124240	10.3196345898	8.1582103806
H	8.0671665648	9.8781890639	2.5247536994
H	2.3625493669	3.8481671943	10.6315451928
H	3.6182101008	8.5831203765	11.3505156420
H	8.4651405192	10.2479596619	4.1022137225
C	3.7904053825	2.9468016450	9.3609524555

C	9.6902803097	4.1034372197	2.7320601810
H	1.6524233260	10.5305314673	3.8932005994
C	8.8710115433	9.4580139782	9.9977928696
H	2.2589518729	9.0838030385	4.5306135418
H	3.2463606909	2.5859085371	11.3656512671
C	3.4904048895	9.9417552162	3.0531052947
H	10.7261588463	9.7826679752	9.0533763426
C	3.7834976586	9.6652146683	9.5186697826
C	4.2441401493	3.6715765306	2.5626023373
C	10.0761967248	10.4952983361	2.7283964033
H	2.8961017326	10.5734587670	4.9878339560
H	10.8601297014	2.1598873461	9.9396785909
C	10.2274922414	3.8658627261	8.8843057719
H	11.2767924941	2.8031234641	2.2136678986
H	9.6550623976	1.8506817140	8.8515763698
H	2.2256897764	8.5946831274	10.4513257326
H	3.1207128956	2.8696661911	4.1640876285
H	8.2148129145	11.4766372772	2.9837590734
N	3.0443861529	9.1788197516	10.7177104885
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N	8.6322965935	10.5216496208	3.1123544853
N	2.8095393810	2.9157443184	10.4836542859
N	9.7401510071	9.5799590013	8.7935117987
N	10.9045678327	3.2876761644	3.0517083874
N	9.9811897223	2.5497919517	9.5411463572
N	2.5142163463	10.0247502775	4.1801366630
I	9.8234477492	13.0652874269	12.4229748140
I	7.2298129881	0.7701747688	2.6825030805
I	13.1097118763	13.7997329578	9.4053965203
I	6.6635246092	12.6710468700	9.6448117517
I	3.6167131452	6.7936953561	5.8340443068
I	9.6187723463	6.7824247905	6.4407092666
I	6.4180886229	6.4507922020	9.2733192356
I	7.1249953239	3.0053571894	11.8719349521
I	12.3797072806	10.3101650873	6.3909002711
I	6.4147691709	10.0728721604	0.1362124633
I	1.2742548637	6.0579012050	9.7733136419
I	12.6478118909	7.2694903010	3.0254844151
I	3.2984247557	6.8677005258	0.3807978444
I	10.2596864378	1.0818720522	5.9737571673
I	6.9260800681	7.0245876345	3.2700385783
I	12.5798571200	9.7358953454	11.1628672256
I	6.7192922132	3.7819370167	6.0595172940
I	0.5494277371	-0.0803056372	3.3259864231
I	3.8145015750	0.3716852145	-0.0031499179
I	10.2586816708	6.1760888195	12.1147268138
I	0.5083675028	3.3610125456	0.5584334282
I	0.8763085221	3.3246880519	6.1071223031
I	3.2359791902	12.4936326121	6.6512308501
I	6.8576565635	9.7537849222	6.2879197347

(MA)₃Bi₂I₉

Bi	5.403404	11.394726	7.593128
Bi	5.403404	3.337954	14.124978
Bi	5.403404	11.394726	3.265925
Bi	5.403404	3.337954	18.452181
Bi	0.000000	4.028386	7.593128
Bi	0.000000	10.704294	14.124978
Bi	0.000000	4.028386	3.265925
Bi	0.000000	10.704294	18.452181
H	6.279815	3.933139	5.429526
H	6.279815	10.799541	16.288579
H	4.526993	10.799541	16.288579
H	4.526993	3.933139	5.429526
H	7.443962	2.085330	8.911156
H	7.443962	12.647350	12.806950
H	7.443962	2.085330	1.947897
H	7.443962	12.647350	19.770209
H	3.362846	12.647350	12.806950
H	3.362846	2.085330	8.911156
H	3.362846	12.647350	19.770209
H	3.362846	2.085330	1.947897
H	6.587776	0.758645	8.213136
H	6.587776	13.974035	13.504970
H	6.587776	0.758645	2.645917
H	6.587776	13.974035	19.072189
H	4.219032	13.974035	13.504970
H	4.219032	0.758645	8.213136
H	4.219032	13.974035	19.072189
H	4.219032	0.758645	2.645917
H	4.532624	3.929869	9.779403
H	4.532624	10.802811	11.938703
H	4.532624	3.929869	1.079650
H	4.532624	10.802811	20.638456
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H	6.274184	3.929869	9.779403
H	6.274184	10.802811	20.638456
H	6.274184	3.929869	1.079650
H	8.760198	13.335101	5.429526
H	8.760198	1.397579	16.288579
H	2.046610	1.397579	16.288579
H	2.046610	13.335101	5.429526
H	9.614444	0.109854	5.429526
H	9.614444	14.622826	16.288579
H	1.192364	14.622826	16.288579
H	1.192364	0.109854	5.429526
H	0.876411	11.299479	5.429526
H	0.876411	3.433201	16.288579
H	9.930397	3.433201	16.288579
H	9.930397	11.299479	5.429526
H	2.040558	9.451670	8.911156
H	2.040558	5.281010	12.806950

H	2.040558	9.451670	1.947897
H	2.040558	5.281010	19.770209
H	8.766250	5.281010	12.806950
H	8.766250	9.451670	8.911156
H	8.766250	5.281010	19.770209
H	8.766250	9.451670	1.947897
H	1.184372	8.124985	8.213136
H	1.184372	6.607695	13.504970
H	1.184372	8.124985	2.645917
H	1.184372	6.607695	19.072189
H	9.622436	6.607695	13.504970
H	9.622436	8.124985	8.213136
H	9.622436	6.607695	19.072189
H	9.622436	8.124985	2.645917
H	9.936028	11.296209	9.779403
H	9.936028	3.436471	11.938703
H	9.936028	11.296209	1.079650
H	9.936028	3.436471	20.638456
H	0.870780	3.436471	11.938703
H	0.870780	11.296209	9.779403
H	0.870780	3.436471	20.638456
H	0.870780	11.296209	1.079650
H	3.356794	5.968761	5.429526
H	3.356794	8.763919	16.288579
H	7.450014	8.763919	16.288579
H	7.450014	5.968761	5.429526
H	4.211040	7.476194	5.429526
H	4.211040	7.256486	16.288579
H	6.595768	7.256486	16.288579
H	6.595768	7.476194	5.429526
C	5.403404	2.284464	8.918084
C	5.403404	12.448216	12.800022
C	5.403404	2.284464	1.940969
C	5.403404	12.448216	19.777137
C	5.403404	5.790930	5.429526
C	5.403404	8.941750	16.288579
C	0.000000	9.650804	8.918084
C	0.000000	5.081876	12.800022
C	0.000000	9.650804	1.940969
C	0.000000	5.081876	19.777137
C	0.000000	13.157270	5.429526
C	0.000000	1.575410	16.288579
I	2.102021	2.753081	5.429526
I	2.102021	11.979599	16.288579
I	8.704787	11.979599	16.288579
I	8.704787	2.753081	5.429526
I	5.403404	13.915738	5.429526
I	5.403404	0.816942	16.288579
I	3.203451	12.732792	9.133072
I	3.203451	1.999888	12.585034
I	3.203451	12.732792	1.725981
I	3.203451	1.999888	19.992125

I	7.603357	1.999888	12.585034
I	7.603357	12.732792	9.133072
I	7.603357	1.999888	19.992125
I	7.603357	12.732792	1.725981
I	5.403404	8.869795	9.154160
I	5.403404	5.862885	12.563946
I	5.403404	8.869795	1.704893
I	5.403404	5.862885	20.013213
I	7.505425	10.119421	5.429526
I	7.505425	4.613259	16.288579
I	3.301383	4.613259	16.288579
I	3.301383	10.119421	5.429526
I	0.000000	6.549398	5.429526
I	0.000000	8.183282	16.288579
I	8.606855	5.366452	9.133072
I	8.606855	9.366228	12.585034
I	8.606855	5.366452	1.725981
I	8.606855	9.366228	19.992125
I	2.199953	9.366228	12.585034
I	2.199953	5.366452	9.133072
I	2.199953	9.366228	19.992125
I	2.199953	5.366452	1.725981
I	0.000000	1.503455	9.154160
I	0.000000	13.229225	12.563946
I	0.000000	1.503455	1.704893
I	0.000000	13.229225	20.013213
N	5.403404	4.453439	5.429526
N	5.403404	10.279241	16.288579
N	6.563953	1.708217	8.573548
N	6.563953	13.024463	13.144558
N	6.563953	1.708217	2.285505
N	6.563953	13.024463	19.432601
N	4.242855	13.024463	13.144558
N	4.242855	1.708217	8.573548
N	4.242855	13.024463	19.432601
N	4.242855	1.708217	2.285505
N	5.403404	3.448022	9.567238
N	5.403404	11.284658	12.150868
N	5.403404	3.448022	1.291815
N	5.403404	11.284658	20.426291
N	9.648453	13.824801	5.429526
N	9.648453	0.907879	16.288579
N	1.158355	0.907879	16.288579
N	1.158355	13.824801	5.429526
N	0.000000	11.819779	5.429526
N	0.000000	2.912901	16.288579
N	1.160549	9.074557	8.573548
N	1.160549	5.658123	13.144558
N	1.160549	9.074557	2.285505
N	1.160549	5.658123	19.432601
N	9.646259	5.658123	13.144558
N	9.646259	9.074557	8.573548

N 9.646259 5.658123 19.432601
 N 9.646259 9.074557 2.285505
 N 0.000000 10.814362 9.567238
 N 0.000000 3.918318 12.150868
 N 0.000000 10.814362 1.291815
 N 0.000000 3.918318 20.426291
 N 4.245049 6.458461 5.429526
 N 4.245049 8.274219 16.288579
 N 6.561759 8.274219 16.288579
 N 6.561759 6.458461 5.429526

Table S2: Calculated band gaps of all the compounds using PAW pseudopotential :

Compounds	CBM (eV)	VBM (eV)	Band Gaps (eV)	Band gaps obtained through USPP (eV)
(MA) ₃ (Ga _{.25} In _{.75}) ₂ I ₉	3.3392	1.1700	2.17	2.16
(MA) ₃ (Ga _{.50} In _{.50}) ₂ I ₉	2.8966	0.9147	1.98	2.10
(MA) ₃ (Ga _{.75} In _{.25}) ₂ I ₉	2.9973	0.8115	2.19	2.22
(MA) ₃ Ga ₂ I ₉	2.8953	0.6714	2.23	2.31
(MA) ₃ In ₂ I ₉	3.2300	1.1617	2.06	2.03

Table S3: Calculated lattice vectors, crystallographic angles, the reciprocal lattice vectors, and the space group of the relaxed structures:

Compounds	Lattice Vectors (Å)	Crystallographic angles (°)	Reciprocal lattice vectors (Å)	Space group
	a=b=c	$\alpha=\beta=\gamma$	a'=b'=c'	
(MA) ₃ (Ga _{.25} In _{.75}) ₂ I ₉	13.05	90	0.08	P 1
(MA) ₃ (Ga _{.50} In _{.50}) ₂ I ₉	13.05	90	0.08	
(MA) ₃ (Ga _{.75} In _{.25}) ₂ I ₉	13.05	90	0.08	
(MA) ₃ Ga ₂ I ₉	13.05	90	0.08	
(MA) ₃ In ₂ I ₉	13.05	90	0.08	