

Supplementary Material

Rational design of mixed Sn-Ge based hybrid halide perovskites for optoelectronic applications: A first principles study

Tridip Chutia ¹ and Dhruba Jyoti Kalita ^{1, a)}

Department of Chemistry, Gauhati University

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

Table S1: Coordinates of the studied compounds (in Angstroms) optimized by employing PBE functional

DMASnI₃

Sn	0.088027981	4.566108963	0.010440241
Sn	4.368884981	4.599020037	15.021015759
Sn	4.368884981	-0.016455037	7.505287759
Sn	0.088027981	9.181584037	7.526168241
H	5.310495515	8.606567146	1.292490568
H	1.029638515	0.558561854	13.738965432
H	1.029638515	4.024003146	6.223237432
H	5.310495515	5.141125854	8.808218568
H	4.992180271	0.297570182	2.837027641
H	0.711323271	8.867558818	12.194428359
H	0.711323271	4.880135182	4.678700359
H	4.992180271	4.284993818	10.352755641
H	4.744915459	7.688422999	2.725075825
H	0.464058459	1.476706001	12.306380175
H	0.464058459	3.105858999	4.790652175
H	4.744915459	6.059270001	10.240803825
H	4.395345858	9.093518954	12.320833832
H	0.114488858	0.071610046	2.710622168
H	0.114488858	4.510953954	10.226350168
H	4.395345858	4.654175046	4.805105832
H	2.989947036	7.964827875	12.243007414
H	7.270804036	1.200301125	2.788448586
H	7.270804036	3.382262875	10.304176586
H	2.989947036	5.782866125	4.727279414
H	3.361800661	8.839980781	13.764410190
H	7.642657661	0.325148219	1.267045810
H	7.642657661	4.257416781	8.782773810
H	3.361800661	4.907712219	6.248682190
H	2.537615484	0.979177238	11.209945379
H	6.818472484	8.185951762	3.821510621
H	6.818472484	5.561741238	11.337238621

H	2.537615484	3.603387762	3.694217379
H	2.813265221	1.759712131	12.634826237
H	7.094122221	7.405416869	2.396629763
H	7.094122221	6.342277131	9.912357763
H	2.813265221	2.822851869	5.119098237
C	5.348897807	8.533288683	2.383174349
C	1.068040807	0.631840317	12.648281651
C	1.068040807	3.950724683	5.132553651
C	5.348897807	5.214404317	9.898902349
C	3.377186823	8.898642348	12.671929449
C	7.658043823	0.266486652	2.359526551
C	7.658043823	4.316077348	9.875254551
C	3.377186823	4.849051652	5.156201449
I	1.723405085	6.616936997	1.415821101
I	6.004262085	2.548192003	13.615634899
I	6.004262085	2.034371997	6.099906899
I	1.723405085	7.130757003	8.931549101
I	2.312647390	4.562441458	12.631805134
I	6.593504390	4.602687542	2.399650866
I	6.593504390	9.145005458	9.915378866
I	2.312647390	0.020123542	5.116077134
I	6.926987263	6.707779758	13.736128867
I	2.646130263	2.457349242	1.295327133
I	2.646130263	2.125215758	8.811055133
I	6.926987263	7.039913242	6.220400867
N	2.486979145	0.848965882	12.245514059
N	6.767836145	8.316163118	2.785941941
N	6.767836145	5.431529882	10.301669941
N	2.486979145	3.733599118	4.729786059

DMAGeI₃

Ge	0.124100140	4.806150278	-0.096017035
Ge	4.404957140	4.358978722	15.127473035
Ge	4.404957140	0.223586278	7.611745035
Ge	0.124100140	8.941542722	7.419710965
H	5.403468385	8.466379839	1.215362864
H	1.122611385	0.698749161	13.816093136
H	1.122611385	3.883815839	6.300365136
H	5.403468385	5.281313161	8.731090864
H	4.955182349	0.030383198	2.789845723
H	0.674325349	9.134745802	12.241610277
H	0.674325349	4.612948198	4.725882277
H	4.955182349	4.552180802	10.305573723
H	5.023020143	7.403835558	2.605284438
H	0.742163143	1.761293442	12.426171562
H	0.742163143	2.821271558	4.910443562
H	5.023020143	6.343857442	10.121012438
H	4.356718474	8.746629505	12.414128752
H	0.075861474	0.418499495	2.617327248
H	0.075861474	4.164064505	10.133055248
H	4.356718474	5.001064495	4.898400752
H	2.830591078	7.854484087	12.096943208
H	7.111448078	1.310644913	2.934512792

H	7.111448078	3.271919087	10.450240792
H	2.830591078	5.893209913	4.581215208
H	3.173643362	8.473101643	13.737926110
H	7.454500362	0.692027357	1.293529890
H	7.454500362	3.890537643	8.809257890
H	3.173643362	5.274591357	6.222198110
H	2.694206583	0.974079122	11.306815684
H	6.975063583	8.191049878	3.724640316
H	6.975063583	5.556643122	11.240368316
H	2.694206583	3.608485878	3.791087684
H	3.130579167	1.565754601	12.786758678
H	7.411436167	7.599374399	2.244697322
H	7.411436167	6.148319601	9.760425322
H	3.130579167	3.016809399	5.271030678
C	5.463015676	8.358521996	2.302113818
C	1.182158676	0.806607004	12.729342182
C	1.182158676	3.775957996	5.213614182
C	5.463015676	5.389171004	9.817841818
C	3.296348382	8.663666333	12.667628048
C	7.577205382	0.501462667	2.363827952
C	7.577205382	4.081101333	9.879555952
C	3.296348382	5.084027667	5.151900048
I	1.446758861	6.734138116	1.362807520
I	5.727615861	2.430990884	13.668648480
I	5.727615861	2.151573116	6.152920480
I	1.446758861	7.013555884	8.878535520
I	1.999350739	4.673659760	12.781739237
I	6.280207739	4.491469240	2.249716763
I	6.280207739	9.256223760	9.765444763
I	1.999350739	-0.091094760	5.266011237
I	6.894204281	6.577174308	13.641223259
I	2.613347281	2.587954692	1.390232741
I	2.613347281	1.994610308	8.905960741
I	6.894204281	7.170518692	6.125495259
N	2.618507381	0.783207534	12.332929568
N	6.899364381	8.381921466	2.698526432
N	6.899364381	5.365771534	10.214254432
N	2.618507381	3.799357466	4.817201568

DMASn₇₅Ge₂₅I₃

Sn	3.239069620	6.716619961	9.314672275
Sn	3.189038380	6.274440039	2.762433275
Ge	9.700336716	0.032241636	3.924784986
Ge	9.583987284	12.958818364	10.477023986
Sn	9.652792632	6.344966785	3.861161994
Sn	9.631531368	6.646093215	10.413400994
Sn	3.153509948	13.201845448	9.331983266
Sn	3.274598052	-0.210785448	2.779744266
H	12.205870944	1.930243034	5.701003186
H	7.078453056	11.060816966	12.253241186
H	5.719363358	4.487481107	7.527996739
H	0.708744642	8.503578893	0.975758739
H	0.417232366	11.165439250	7.421441448

H	6.010875634	1.825620750	0.869203448
H	7.134367161	8.486002484	5.608349392
H	12.149956839	4.505057516	12.160587392
H	0.694176630	2.174772985	6.619002378
H	5.733931370	10.816287015	0.066764378
H	7.101702982	4.424546908	6.631955200
H	12.182621018	8.566513092	13.184193200
H	12.017641623	10.829030759	6.404443920
H	7.266682377	2.162029241	12.956681920
H	5.758429416	8.643060269	6.505089288
H	0.669678584	4.347999731	-0.047148712
H	0.727243730	3.590225742	4.711803885
H	5.700864270	9.400834258	11.264042885
H	7.181467016	2.841345730	8.406858898
H	12.102856984	10.149714270	1.854619898
H	11.959690068	9.419802661	8.324213375
H	7.324633932	3.571257339	1.771974375
H	5.713144918	10.129480625	4.656678839
H	0.714963082	2.861579375	11.208917839
H	12.001084251	4.275128717	5.208655365
H	7.283239749	8.715931283	11.760894365
H	5.674358980	2.087929134	7.784101386
H	0.753749020	10.903130866	1.231862386
H	0.750897759	8.834040453	7.923545171
H	5.677210241	4.157019547	1.371306171
H	7.257795174	10.855922326	5.210312542
H	12.026528826	2.135137674	11.762551542
H	0.604052849	4.564426158	6.217684741
H	5.824055151	8.426633842	12.769922741
H	7.184273054	2.011366526	6.814268617
H	12.100050946	10.979693474	0.262030617
H	12.226494928	8.457288619	6.832385435
H	7.057829072	4.533771381	0.280147435
H	5.769942612	11.049171868	6.199435171
H	0.658165388	1.941888132	12.751673171
H	10.819189672	3.216247104	7.199425092
H	8.465134328	9.774812896	0.647187092
H	4.461866906	3.258788684	5.878286632
H	1.966241094	9.732271316	12.430524632
H	1.985073774	9.962321393	6.032721494
H	4.443034226	3.028738607	12.584959494
H	8.443280668	9.740554123	7.185949415
H	10.841043332	3.250505877	0.633711415
H	11.677295996	1.891654057	8.063915605
H	7.607028004	11.099405943	1.511676605
H	5.245188359	4.715275120	5.169584158
H	1.182919641	8.275784880	11.721823158
H	1.121667739	11.236782091	5.103310027
H	5.306440261	1.754277909	11.655549027
H	7.599418104	8.370360082	7.983662723
H	11.684905896	4.620699918	1.431423723
H	12.273885501	3.584051197	8.178906984
H	7.010438499	9.407008803	1.626667984
H	5.963748547	3.086351268	4.912082439

H	0.464359453	9.904708732	11.464321439
H	0.629083916	9.514910623	4.945471062
H	5.799024084	3.476149377	11.497710062
H	6.953788121	10.042440241	8.141087273
H	12.330535879	2.948619759	1.588848273
C	0.090060061	3.855355070	5.562515517
C	6.338047939	9.135704930	12.114754517
C	6.593537413	2.613555575	7.511262088
C	12.690786587	10.377504425	0.959023088
C	12.659973368	9.195094231	7.513162555
C	6.624350632	3.795965769	0.960923555
C	6.323870983	10.385590200	5.528823879
C	0.104237017	2.605469800	12.081062879
C	11.790806456	2.842581184	7.534960621
C	7.493517544	10.148478816	0.982722621
C	5.413191479	3.726728388	5.608088726
C	1.014916521	9.264331612	12.160326726
C	1.021514259	10.279376159	5.623294334
C	5.406593741	2.711683841	12.175532334
C	7.472139554	9.336256112	7.485512103
C	11.812184446	3.654803888	0.933274103
I	2.681146353	3.922337239	8.717543919
I	3.746961647	9.068722761	2.165305919
I	9.144283728	2.691391544	4.213174700
I	10.140040272	10.299668456	10.765412700
I	10.142259737	9.169401809	4.365915159
I	9.142064263	3.821658191	10.918153159
I	3.785757925	10.410810723	8.836666545
I	2.642350075	2.580249277	2.284428545
I	6.023875980	6.027156832	9.791467957
I	0.404232020	6.963903168	3.239228957
I	12.356481914	0.429846494	3.429728281
I	6.927842086	12.561213506	9.981967281
I	6.841088592	6.902469655	3.361427288
I	12.443235408	6.088590345	9.913666288
I	0.347155480	12.569373565	9.687480108
I	6.080952520	0.421686435	3.135241108
I	3.632500583	7.242604365	6.433618725
I	2.795607417	5.748455635	12.985857725
I	9.924672557	12.503345765	6.609571776
I	9.359651443	0.487714235	0.057332776
I	9.186576919	5.839532983	6.752487186
I	10.097747081	7.151527017	0.200248186
I	2.820667821	0.702139246	6.433728843
I	3.607440179	12.288920754	12.985967843
N	12.649085221	2.620092468	6.339515363
N	6.635238779	10.370967532	12.891754363
N	6.225818930	3.892516004	6.843546209
N	0.202289070	9.098543996	0.291307209
N	0.066187704	10.448366419	6.752090048
N	6.361920296	2.542693581	0.199851048
N	6.649926673	9.131749245	6.262497669
N	12.634397327	3.859310755	12.814736669

DMASn₅₀Ge₅₀I₃

Sn	3.289688433	6.748049200	9.318412138
Sn	3.138419567	6.243010800	2.766173138
Ge	9.689635822	0.063789481	3.986102623
Ge	9.594688178	12.927270519	10.538341623
Ge	9.594688178	6.559319481	3.986102623
Ge	9.689635822	6.431740519	10.538341623
Sn	3.138419567	13.243579200	9.318412138
Sn	3.289688433	-0.252519200	2.766173138
H	12.124651452	2.001245749	5.709108571
H	7.159672548	10.989814251	12.261346571
H	5.977569505	4.641699838	7.447436057
H	0.450538495	8.349360162	0.895198057
H	0.450538495	11.137229838	7.447436057
H	5.977569505	1.853830162	0.895198057
H	7.159672548	8.496775749	5.709108571
H	12.124651452	4.494284251	12.261346571
H	0.653024692	2.185951113	6.588379669
H	5.775083308	10.805108887	0.036141669
H	7.255955791	4.434328291	6.429080990
H	12.028368209	8.556731709	12.981318990
H	12.028368209	10.929858291	6.429080990
H	7.255955791	2.061201709	12.981318990
H	5.775083308	8.681481113	6.588379669
H	0.653024692	4.309578887	0.036141669
H	0.703154405	3.581885799	4.669465958
H	5.724953595	9.409174201	11.221704958
H	7.402241507	2.973121233	8.310761621
H	11.882082493	10.017938767	1.758522621
H	11.882082493	9.468651233	8.310761621
H	7.402241507	3.522408767	1.758522621
H	5.724953595	10.077415799	4.669465958
H	0.703154405	2.913644201	11.221704958
H	12.032522684	4.357484901	5.205928322
H	7.251801316	8.633575099	11.758167322
H	5.815733659	2.268186274	7.863234808
H	0.612374341	10.722873726	1.310995808
H	0.612374341	8.763716274	7.863234808
H	5.815733659	4.227343726	1.310995808
H	7.251801316	10.853014901	5.205928322
H	12.032522684	2.138045099	11.758167322
H	0.676782231	4.569694327	6.172290784
H	5.751325769	8.421365673	12.724528784
H	7.239512939	2.038204483	6.788368268
H	12.044811061	10.952855517	0.236130268
H	12.044811061	8.533734483	6.788368268
H	7.239512939	4.457325517	0.236130268
H	5.751325769	11.065224327	6.172290784
H	0.676782231	1.925835673	12.724528784
H	10.841572161	3.351434621	7.232386289
H	8.442751839	9.639625379	0.680148289
H	4.507432223	3.358648757	6.017763614
H	1.920675777	9.632411243	12.570001614

H	1.920675777	9.854178757	6.017763614
H	4.507432223	3.136881243	12.570001614
H	8.442751839	9.846964621	7.232386289
H	10.841572161	3.144095379	0.680148289
H	11.671051275	2.008785078	8.089873260
H	7.613272725	10.982274922	1.537634260
H	5.259534312	4.734005016	5.141096961
H	1.168573688	8.257054984	11.693335961
H	1.168573688	11.229535016	5.141096961
H	5.259534312	1.761524984	11.693335961
H	7.613272725	8.504315078	8.089873260
H	11.671051275	4.486744922	1.537634260
H	12.337349798	3.676220805	8.163345594
H	6.946974202	9.314839195	1.611106594
H	5.889237948	3.065851971	4.912403530
H	0.538870052	9.925208029	11.464642530
H	0.538870052	9.561381971	4.912403530
H	5.889237948	3.429678029	11.464642530
H	6.946974202	10.171750805	8.163345594
H	12.337349798	2.819309195	1.611106594
C	0.105840451	3.886575805	5.535464593
C	6.322267549	9.104484195	12.087703593
C	6.735609084	2.719383247	7.480592036
C	12.548714916	10.271676753	0.928353036
C	12.548714916	9.214913247	7.480592036
C	6.735609084	3.776146753	0.928353036
C	6.322267549	10.382105805	5.535464593
C	0.105840451	2.608954195	12.087703593
C	11.808257899	2.945948866	7.543539849
C	7.476066101	10.045111134	0.991301849
C	5.440756036	3.768736349	5.621734019
C	0.987351964	9.222323651	12.173972019
C	0.987351964	10.264266349	5.621734019
C	5.440756036	2.726793651	12.173972019
C	7.476066101	9.441478866	7.543539849
C	11.808257899	3.549581134	0.991301849
I	2.645418922	3.972958327	8.774141622
I	3.782689078	9.018101673	2.221903622
I	9.199628104	2.740444353	4.217965177
I	10.084695896	10.250615647	10.770203177
I	10.084695896	9.235974353	4.217965177
I	9.199628104	3.755085647	10.770203177
I	3.782689078	10.468488327	8.774141622
I	2.645418922	2.522571673	2.221903622
I	6.089292383	6.073078542	9.690925689
I	0.338815617	6.917981458	3.138686689
I	12.354632391	0.359640574	3.464524263
I	6.929691609	12.631419426	10.016763263
I	6.929691609	6.855170574	3.464524263
I	12.354632391	6.135889426	10.016763263
I	0.338815617	12.568608542	9.690925689
I	6.089292383	0.422451458	3.138686689
I	3.615446809	7.279489339	6.427810164
I	2.812661191	5.711570661	12.980049164

I	9.945954796	12.566852285	6.680173838
I	9.338369204	0.424207715	0.127934838
I	9.338369204	6.071322285	6.680173838
I	9.945954796	6.919737715	0.127934838
I	2.812661191	0.783959339	6.427810164
I	3.615446809	12.207100661	12.980049164
N	12.621837391	2.671606967	6.327554599
N	6.662486609	10.319453033	12.879793599
N	6.381057499	3.972642294	6.757290094
N	0.047050501	9.018417706	0.205051093
N	0.047050501	10.468172294	6.757290094
N	6.381057499	2.522887706	0.205051093
N	6.662486609	9.167136967	6.327554599
N	12.621837391	3.823923033	12.879793599

DMASn₂₅Ge₇₅I₃

Ge	3.395717927	6.536290634	9.239056998
Ge	3.032390073	6.454769366	2.686817998
Ge	9.696055626	-0.003955493	4.019453707
Ge	9.588268374	12.995015493	10.571692707
Ge	9.588835517	6.616263391	3.950366974
Ge	9.695488483	6.374796609	10.502605974
Sn	3.183554872	13.213490650	9.251701873
Sn	3.244553128	-0.222430650	2.699462873
H	12.065349244	2.074232082	5.641183373
H	7.218974756	10.916827918	12.193421373
H	6.035346959	4.643046847	7.342729048
H	0.392761041	8.348013153	0.790491048
H	0.488741807	11.070695602	7.487599450
H	5.939366193	1.920364398	0.935361450
H	6.884909009	8.407645275	5.774829109
H	12.399414991	4.583414725	12.327067109
H	0.630468514	2.125980951	6.478946228
H	5.797639486	10.865079049	-0.073291772
H	7.296191315	4.342882360	6.326615322
H	11.988132685	8.648177640	12.878853322
H	12.052746319	10.905953496	6.483512431
H	7.231577681	2.085106504	13.035750431
H	5.610633632	8.768764768	6.758170449
H	0.817474368	4.222295232	0.205932449
H	0.696298744	3.634331810	4.639717219
H	5.731809256	9.356728190	11.191956219
H	7.395019551	2.952849670	8.270148564
H	11.889304449	10.038210330	1.717909564
H	11.881167375	9.424156637	8.341475636
H	7.403156625	3.566903363	1.789236636
H	5.549285612	10.095532740	4.784951947
H	0.878822388	2.895527260	11.337190947
H	12.091234940	4.458012914	5.289274272
H	7.193089060	8.533047086	11.841513272
H	5.777639123	2.300095868	7.850666557
H	0.650468877	10.690964132	1.298427557
H	0.593594367	8.684461327	7.874156546

H	5.834513633	4.306598673	1.321917546
H	7.187971846	10.716985502	5.170708447
H	12.096352154	2.274074498	11.722947447
H	0.783856218	4.525726146	6.197033115
H	5.644251782	8.465333854	12.749271115
H	7.186325817	1.971633489	6.780529925
H	12.097998183	11.019426511	0.228291925
H	12.014188929	8.508514204	6.805788131
H	7.270135071	4.482545796	0.253550131
H	5.796301301	11.124774158	6.236900143
H	0.631806699	1.866285842	12.789138143
H	10.920881232	3.425202419	7.277132096
H	8.363442768	9.565857581	0.724894096
H	4.512615995	3.346516323	5.969840088
H	1.915492005	9.644543677	12.522078088
H	1.911705403	9.763643037	6.024457338
H	4.516402597	3.227416963	12.576695338
H	8.415399119	9.692763988	7.133998938
H	10.868924881	3.298296012	0.581760938
H	11.657862036	1.960496449	8.012985292
H	7.626461964	11.030563551	1.460746292
H	5.295017504	4.680260797	5.048630777
H	1.133090496	8.310799203	11.600869777
H	1.192158759	11.177098854	5.183258920
H	5.235949241	1.813961146	11.735497920
H	7.553419963	8.452489156	8.107910587
H	11.730904037	4.538570844	1.555671587
H	12.459669308	3.563336555	8.187204184
H	6.824654692	9.427723445	1.634965184
H	5.879053652	2.989658469	4.866202475
H	0.549054348	10.001401531	11.418441475
H	0.503647954	9.534760171	4.932437782
H	5.924460046	3.456299829	11.484676782
H	7.038343366	10.172497991	8.176385409
H	12.245980634	2.818562009	1.624146409
C	0.148896745	3.915765507	5.546225728
C	6.279211255	9.075294493	12.098464728
C	6.715097559	2.696108080	7.450788451
C	12.569226441	10.294951920	0.898549451
C	12.539471383	9.165411744	7.505707530
C	6.744852617	3.825648256	0.953468530
C	6.241778356	10.363827593	5.589560901
C	0.186329644	2.627232407	12.141799901
C	11.858483437	2.923105400	7.533663098
C	7.425840563	10.067954600	0.981425098
C	5.452156513	3.724196931	5.556224685
C	0.975951487	9.266863069	12.108462685
C	0.986146031	10.208317650	5.647260111
C	5.441961969	2.782742350	12.199498111
C	7.449291376	9.381723529	7.540851471
C	11.835032624	3.609336471	0.988613471
I	2.725212144	3.915773687	8.980151204
I	3.702895856	9.075286313	2.427913204
I	9.201323691	2.675843871	4.270936889

I	10.083000309	10.315216129	10.823174889
I	10.103040066	9.282199694	4.178032916
I	9.181283934	3.708860306	10.730270916
I	3.761958308	10.418260823	8.723643029
I	2.666149692	2.572799177	2.171405029
I	6.070188361	6.075341422	9.593008695
I	0.357919639	6.915718578	3.040769695
I	12.353227220	0.326368895	3.453712646
I	6.931096780	12.664691105	10.005951646
I	6.905829247	6.899063321	3.545247531
I	12.378494753	6.091996679	10.097486531
I	0.372813389	12.615061739	9.670808841
I	6.055294611	0.375998261	3.118569841
I	3.496122634	7.088141969	6.556103485
I	2.931985366	5.902918031	13.108342485
I	9.958096279	12.503957612	6.713290369
I	9.326227721	0.487102388	0.161051369
I	9.417713248	6.056908063	6.636375304
I	9.866610752	6.934151937	0.084136304
I	2.797583626	0.786613669	6.367443120
I	3.630524374	12.204446331	12.919682120
N	12.620505370	2.676587395	6.278133980
N	6.663818630	10.314472605	12.830372980
N	6.407577747	3.933085637	6.678847890
N	0.020530253	9.057974363	0.126608890
N	0.063574767	10.418595528	6.796208549
N	6.364533233	2.572464472	0.243969549
N	6.514063596	9.147888321	6.406124224
N	12.770260404	3.843171679	12.958363224

Table S2: Validation of the reference compound (DMAPbI₃) with different functionals

Functionals	VBM (eV)	CBM (eV)	Band Gap (eV)
PBE	1.3008	3.9241	2.62
PBEsol	1.1812	4.4717	3.29
PBE0	0.4716	5.2422	4.77
HSE06	0.8454	4.9010	4.05

Table S3: Calculated lattice parameters of the studied OIHPs in Å.

Compounds	Theoretical			Experimental		
	a	b	c	a	b	c
DMASnI ₃	8.56	9.17	15.00	8.28	8.78	14.63
DMAGeI ₃	8.56	9.16	15.03			
DMASn _{0.75} Ge _{0.25} I ₃	12.86	12.99	13.10			
DMASn _{0.50} Ge _{0.50} I ₃	12.86	12.99	13.10			
DMASn _{0.25} Ge _{0.75} I ₃	12.86	12.99	13.10			

