

Superalkali-alkaline earthide ion pairs of $\delta^+(\text{AM-HMHC})-\text{AM}'\delta^-$ (AM = Li, Na & K; AM' = Be, Mg & Ca) possessing large NLO responses and excellent electronic stabilities and alkalide characteristics: A DFT study

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Chair (Li-HMHC)-Be				Boat (Li-HMHC)-Be			
N	1.37369510	-2.09617415	-0.28953302	N	-2.84249550	0.05536545	-0.81448615
N	3.48730925	0.00021800	0.03130300	N	-1.19521060	2.27063780	0.60607449
N	1.37342910	2.09626415	-0.28952602	N	1.86982309	2.16735840	0.32204064
N	-1.64374412	2.24976316	0.40901203	N	1.75464213	-0.05913342	-1.42505134
N	-3.20654423	-0.00009600	-0.55131604	N	1.74461236	-2.25851601	0.36421592
N	-1.64350112	-2.24983116	0.40885503	N	-1.29681515	-2.20337393	0.58843523
C	0.89140807	-1.94864314	-1.65278812	C	-2.81358262	0.07386261	-2.25742781
C	4.26089730	0.00036800	1.26713409	C	-1.52116066	2.01443115	1.99637697
C	0.89098006	1.94821414	-1.65267012	C	3.16401702	2.00428182	0.96708443
C	-0.78461405	-3.38630225	0.17361901	C	-2.47875219	-2.36166450	-0.24437151
C	0.69758805	-3.17250623	0.45280503	C	-3.42565012	-1.16315471	-0.28868827
C	2.81087120	-2.36086217	-0.22893002	C	-3.36433573	1.28417183	-0.25079222
C	3.68703526	-1.22404109	-0.73084005	C	-2.37809231	2.45123451	-0.22218180
C	3.68683427	1.22439909	-0.73101105	C	-0.31757519	3.42275351	0.48511057
C	2.81057020	2.36118317	-0.22919202	C	1.10988802	3.22175083	0.98415741
C	-1.68699612	1.87242514	1.80558513	C	0.35311923	-0.01093973	-1.80688787
C	-2.78996020	0.00010100	-1.92746114	C	3.05482297	-2.15043628	0.98705141
C	-1.68711312	-1.87240913	1.80539213	C	-1.61537530	-1.81613478	1.94863522
C	0.69725605	3.17269723	0.45259703	C	2.00786563	2.37336893	-1.11008942
C	-0.78499106	3.38627224	0.17348501	C	2.49301553	1.12134896	-1.83354956
C	-2.95519721	2.44774117	-0.17437901	C	2.40509102	-1.29533035	-1.81832074
C	-3.86012928	1.21400709	-0.12975001	C	1.84373475	-2.49701012	-1.06560272
C	-3.85997728	-1.21440009	-0.13009001	C	0.94070325	-3.25686962	1.05971057
C	-2.95481021	-2.44795717	-0.17481101	C	-0.49290480	-3.41251134	0.56123798
H	-0.16950401	-1.67041812	-1.63369312	H	-2.31611743	-0.82401402	-2.65051105
H	1.02042207	-2.87051421	-2.25968016	H	-3.83507852	0.11622237	-2.69991081
H	1.42988910	-1.13812608	-2.16105216	H	-2.25164288	0.94205039	-2.62969015
H	5.35198640	0.00050600	1.05805008	H	-2.06610810	2.86723005	2.46054148
H	4.01151429	-0.87496506	1.88025513	H	-0.60967229	1.81254570	2.57563115
H	4.01127729	0.87568006	1.88019113	H	-2.14112849	1.11731817	2.09489818
H	1.42943710	1.13753008	-2.16069616	H	3.80586821	2.90299044	0.84390784
H	1.01987007	2.86986620	-2.25992216	H	3.70028692	1.13953617	0.55153001
H	-0.16991001	1.66993512	-1.63332612	H	3.01814771	1.80467411	2.03828730
H	-0.91301107	-3.70516927	-0.87295606	H	-3.08832390	-3.23397981	0.09116209
H	-1.08961208	-4.26471631	0.79061606	H	-2.14445242	-2.60219276	-1.26811573
H	0.87067706	-2.99092122	1.52575411	H	-4.31659050	-1.47646640	-0.87787829
H	1.17998608	-4.14471230	0.21504602	H	-3.80225651	-0.96736384	0.72457691
H	3.06502422	-3.27937124	-0.80274706	H	-3.71325603	1.08246619	0.77119781
H	3.06025322	-2.57236518	0.82251606	H	-4.26342129	1.63731885	-0.80525676
H	4.74418334	-1.55936411	-0.69872305	H	-2.04240161	2.66540914	-1.25061492
H	3.46792225	-1.02460907	-1.78962213	H	-2.95545487	3.34917071	0.10226165
H	3.46766725	1.02480607	-1.78975213	H	-0.30468286	3.73727159	-0.56949385
H	4.74394234	1.55985911	-0.69901305	H	-0.72978763	4.29551216	1.04229674
H	3.06008122	2.57294818	0.82217106	H	1.10016383	2.98374854	2.05855488
H	3.06449822	3.27961024	-0.80324106	H	1.62924006	4.20125058	0.88573150
H	-0.69040405	1.56842311	2.16125616	H	-0.12972121	0.87792738	-1.37978282
H	-2.06346915	2.69633819	2.45318317	H	0.21871195	-0.01036827	-2.90950247

H	-2.33745917	1.00280107	1.94228214	H	-0.19257535	-0.85842340	-1.37129986
H	-3.64738626	0.00005600	-2.64047019	H	3.65116720	-3.08045642	0.86684153
H	-2.17172016	0.88202507	-2.14173615	H	3.62581450	-1.31740058	0.55327824
H	-2.17146916	-0.88160506	-2.14191615	H	2.93458066	-1.93123891	2.05760824
H	-2.33743317	-1.00263807	1.94182914	H	-2.13197517	-0.85097276	1.96515274
H	-2.06393215	-2.69621319	2.45292617	H	-2.25631541	-2.56895377	2.46082395
H	-0.69056905	-1.56859211	2.16134015	H	-0.69643338	-1.67128371	2.53309729
H	0.87044506	2.99139822	1.52557811	H	1.03399866	2.66317140	-1.52300618
H	1.17952109	4.14490230	0.21457002	H	2.70305736	3.20992560	-1.34140310
H	-0.91350106	3.70491826	-0.87314306	H	3.55801280	0.94869032	-1.61656272
H	-1.09002508	4.26477831	0.79033706	H	2.42387926	1.29790833	-2.92914520
H	-3.50976825	3.28063623	0.31916402	H	2.31068194	-1.48673456	-2.90942425
H	-2.81493520	2.76368820	-1.22140209	H	3.48201840	-1.19291197	-1.61657984
H	-4.76677334	1.44825410	-0.73668605	H	2.47303019	-3.38517586	-1.29414185
H	-4.22218030	1.06451408	0.89904007	H	0.84377452	-2.72097430	-1.45670848
H	-4.22221730	-1.06518408	0.89867307	H	1.41723212	-4.26077366	0.99666635
H	-4.76648334	-1.44868110	-0.73721705	H	0.93964704	-2.98124407	2.12535793
H	-2.81430520	-2.76368820	-1.22186809	H	-0.95986330	-4.21686794	1.17515334
H	-3.50931325	-3.28104123	0.31849302	H	-0.49142503	-3.80244048	-0.46820825
Li	1.35363010	0.00005200	0.71033405	Li	1.09937620	-0.01864663	0.74770250
Be	1.35836810	-0.00086500	3.45771825	Be	1.31009423	0.00463868	3.57806368

Chair (Li-HMHC)-Mg				Boat (Li-HMHC)-Mg			
N	1.29702616	-2.09143070	-0.50834325	N	2.99098710	0.01953861	-0.68105892
N	3.42953917	0.00070917	-0.29317725	N	1.20780405	-2.27005903	0.49046715
N	1.29654817	2.09247222	-0.50725755	N	-1.82384906	-2.08957977	-0.16464932
N	-1.68427471	2.25050627	0.32832595	N	-1.49548100	0.19683474	-1.80366010
N	-3.29064325	0.00008247	-0.56154161	N	-1.70918603	2.23945346	0.14937904
N	-1.68401639	-2.25075885	0.32646238	N	1.26207239	2.15452371	0.65176441
C	0.74793591	-1.93819651	-1.84618321	C	3.13468387	0.06070248	-2.11679273
C	4.27676106	0.00067707	0.89379793	C	1.41351472	-2.19564355	1.92609409
C	0.74705549	1.94007191	-1.84502934	C	-3.18025282	-1.95343619	0.34909982
C	-0.83673404	-3.38658418	0.04880004	C	2.52915712	2.39566867	-0.02199916
C	0.65702299	-3.17365780	0.25848188	C	3.50084508	1.21694776	-0.04165504
C	2.73560233	-2.35902886	-0.52011999	C	3.44250104	-1.23190723	-0.10575988
C	3.58682990	-1.22395852	-1.06622138	C	2.46062532	-2.39480789	-0.24261138
C	3.58642790	1.22563519	-1.06588742	C	0.32574444	-3.38084031	0.16474855
C	2.73507700	2.36036379	-0.51926011	C	-1.14432421	-3.18717687	0.51988180
C	-1.66284636	1.87604174	1.72579345	C	-0.06729189	0.14409002	-2.06603087
C	-2.94592028	0.00089321	-1.95762531	C	-3.08853610	2.09643107	0.59229204
C	-1.66309169	-1.87732340	1.72420761	C	1.42155791	1.57782289	1.97184806
C	0.65652294	3.17404700	0.26043921	C	-1.82178909	-2.23660328	-1.61290576
C	-0.83733036	3.38672337	0.05123339	C	-2.21378395	-0.94892881	-2.32941112
C	-3.02168679	2.44770857	-0.19404133	C	-2.09197889	1.46765624	-2.17227890
C	-3.92314621	1.21386862	-0.10740948	C	-1.62303171	2.59461462	-1.25838957
C	-3.92301226	-1.21430850	-0.10883249	C	-1.00370978	3.17609008	1.01829686
C	-3.02122817	-2.44784252	-0.19645338	C	0.47445555	3.37349247	0.69755899

H	-0.31100889	-1.66162088	-1.77248157	H	2.69035936	0.97894793	-2.52661934
H	0.84766852	-2.85741317	-2.46203964	H	4.20121190	0.02874377	-2.43616390
H	1.25979014	-1.12534048	-2.37748630	H	2.61862490	-0.78608728	-2.59107967
H	5.35313774	0.00101488	0.61900018	H	1.88237802	-3.12185240	2.32649400
H	4.06454626	-0.87566295	1.51981406	H	0.45850185	-2.03188226	2.44478915
H	4.06406285	0.87661863	1.52020738	H	2.05292999	-1.34807836	2.19482020
H	1.25887715	1.12769428	-2.37708681	H	-3.79833211	-2.84948289	0.12842920
H	0.84641168	2.85975287	-2.46025042	H	-3.67695678	-1.07623619	-0.08806782
H	-0.31181906	1.66326623	-1.77116748	H	-3.14673629	-1.79333343	1.43699719
H	-1.01382998	-3.70222134	-0.99156632	H	3.07605608	3.24521557	0.45043053
H	-1.11240240	-4.26676798	0.67667599	H	2.31089995	2.71284796	-1.05676164
H	0.88255212	-2.99925182	1.32311713	H	4.43491959	1.57405184	-0.52893687
H	1.12798652	-4.14346191	-0.00897272	H	3.78784745	0.97508445	0.99075772
H	2.95828286	-3.27798838	-1.10562806	H	3.66534295	-1.07018969	0.95783959
H	3.03660682	-2.56993795	0.51809466	H	4.40224783	-1.56588063	-0.56116394
H	4.64339305	-1.56071531	-1.08897628	H	2.21734040	-2.53225548	-1.30895533
H	3.31351629	-1.02324723	-2.11200283	H	3.00633979	-3.31732019	0.06549280
H	3.31293252	1.02517203	-2.11166691	H	0.42540944	-3.59773769	-0.90915714
H	4.64292227	1.56261125	-1.08876466	H	0.65800020	-4.31112955	0.67909789
H	3.03625688	2.57095340	0.51896619	H	-1.24816169	-3.00686072	1.60109425
H	2.95745085	3.27957960	-1.10447985	H	-1.65953315	-4.15133409	0.31414053
H	-0.64859530	1.57618361	2.03458634	H	0.36828696	-0.76806817	-1.63694206
H	-2.00983881	2.69981710	2.38961173	H	0.16327819	0.18497007	-3.15172386
H	-2.30304020	1.00445050	1.89503563	H	0.44510973	0.96683568	-1.55059647
H	-3.83916760	0.00116351	-2.62504014	H	-3.65905102	3.04438525	0.49069339
H	-2.33975416	0.88280969	-2.20397612	H	-3.60639066	1.31956575	0.01263272
H	-2.33955417	-0.88061377	-2.20495859	H	-3.09746288	1.77084764	1.64373845
H	-2.30344938	-1.00593721	1.89388076	H	1.91651814	0.60396241	1.90480357
H	-2.01014515	-2.70162363	2.38732975	H	2.01005893	2.23220308	2.65383731
H	-0.64898700	-1.57754545	2.03351724	H	0.43817354	1.38087982	2.42640374
H	0.88236334	2.99895461	1.32489698	H	-0.81698310	-2.52879330	-1.94052304
H	1.12718917	4.14413408	-0.00651893	H	-2.50252855	-3.05080453	-1.94276475
H	-1.01472781	3.70298902	-0.98889337	H	-3.29092375	-0.76145559	-2.20620980
H	-1.11307519	4.26643257	0.67974702	H	-2.04425876	-1.08521765	-3.41948379
H	-3.55283651	3.28056325	0.32427084	H	-1.86563002	1.74608909	-3.22397260
H	-2.92981354	2.76334269	-1.24643307	H	-3.18530330	1.36244475	-2.11130142
H	-4.85780548	1.44872414	-0.66973451	H	-2.21008210	3.50990459	-1.48953837
H	-4.23554055	1.06313421	0.93729371	H	-0.57860026	2.82898915	-1.49783399
H	-4.23574462	-1.06472510	0.93593250	H	-1.48296275	4.17964428	0.98879364
H	-4.85745617	-1.44878347	-0.67166787	H	-1.12111886	2.80272426	2.04803758
H	-2.92898426	-2.76242464	-1.24913046	H	0.87768981	4.08388080	1.45517044
H	-3.55229330	-3.28133937	0.32091222	H	0.58392213	3.89077931	-0.26815928
Li	1.33321518	0.00039980	0.47997878	Li	-1.06304108	0.03426344	0.41056713
Mg	1.49496556	-0.00464872	3.72505627	Mg	-1.69567164	-0.49765022	3.82267910

Chair (Li-HMHC)-Ca				Boat (Li-HMHC)-Ca			
N	1.17389062	-2.08486062	-0.79754257	N	3.19071525	0.08428375	0.06965702

N	3.32587405	0.00181371	-0.76420174	N	1.18219468	-2.24704040	0.61881393
N	1.17276243	2.08743833	-0.79421074	N	-1.51729013	-2.09871618	-0.92298750
N	-1.73044522	2.24986091	0.27609460	N	-0.75566195	0.21298911	-2.35837692
N	-3.40611198	-0.00002284	-0.47435361	N	-1.59631948	2.19593635	-0.51203873
N	-1.72955426	-2.25066527	0.27170231	N	1.08384672	2.14985653	0.82191367
C	0.51469506	-1.92295486	-2.08411197	C	3.76250345	0.14523991	-1.25438359
C	4.28225440	0.00138453	0.33658697	C	0.91739203	-2.20179633	2.04665487
C	0.51330829	1.92781038	-2.08093425	C	-2.96680972	-1.98533433	-0.81711529
C	-0.90800073	-3.38558165	-0.07774415	C	2.48975822	2.43943154	0.58021503
C	0.59804409	-3.17367786	0.01056393	C	3.45454894	1.28390791	0.84088179
C	2.60605855	-2.35590579	-0.93268022	C	3.47223493	-1.16436297	0.75001542
C	3.41041214	-1.22290966	-1.54932852	C	2.60437695	-2.34490150	0.31609396
C	3.40954341	1.22764650	-1.54767425	C	0.46660744	-3.35792177	0.00913869
C	2.60477650	2.35937019	-0.92922974	C	-1.04664243	-3.20137414	-0.08757015
C	-1.58807596	1.87229135	1.66503399	C	0.68777362	0.17585908	-2.19203662
C	-3.18200585	0.00153750	-1.89494080	C	-3.04267718	2.02482484	-0.51842342
C	-1.58761322	-1.87572700	1.66139190	C	0.84452381	1.49499395	2.09188666
C	0.59666823	3.17443360	0.01617979	C	-1.09724614	-2.22401870	-2.31178764
C	-0.90949016	3.38583362	-0.07132411	C	-1.27472688	-0.92622990	-3.09214914
C	-3.10775205	2.44755521	-0.12953537	C	-1.23576311	1.48814834	-2.85951012
C	-3.99831662	1.21334404	0.03248123	C	-1.08831294	2.59104886	-1.81760025
C	-3.99784926	-1.21471605	0.02986765	C	-1.21207617	3.12561049	0.54649358
C	-3.10669487	-2.44818537	-0.13457351	C	0.28896704	3.35746077	0.68853136
H	-0.53324291	-1.64312625	-1.92042112	H	3.44441347	1.06038173	-1.77394791
H	0.55937762	-2.83959974	-2.70993442	H	4.87600328	0.13651934	-1.23521954
H	0.98292690	-1.10967127	-2.65317680	H	3.43284897	-0.70509388	-1.86812026
H	5.32789804	0.00215613	-0.03881158	H	1.17076621	-3.16273581	2.54690368
H	4.12992321	-0.87530467	0.97973810	H	-0.14251113	-1.96913587	2.23422183
H	4.12912047	0.87688881	0.98115973	H	1.49449930	-1.40881278	2.53420819
H	0.98178778	1.11591355	-2.65177038	H	-3.48166759	-2.89559880	-1.19120843
H	0.55740149	2.84574879	-2.70489773	H	-3.33294189	-1.12331814	-1.39177076
H	-0.53445618	1.64716221	-1.91754506	H	-3.24240841	-1.80952462	0.23473767
H	-1.16978976	-3.69754508	-1.10117861	H	2.83754486	3.28576346	1.21740397
H	-1.13168036	-4.26783629	0.56767783	H	2.59311573	2.78295679	-0.46421004
H	0.91099078	-3.00841095	1.05460439	H	4.48134801	1.67006106	0.65790622
H	1.04499667	-4.14099750	-0.30263980	H	3.42665746	1.03332422	1.91012230
H	2.77494455	-3.27477813	-1.53588634	H	3.35758891	-1.00856483	1.83155725
H	2.99406281	-2.56826141	0.07618660	H	4.53194833	-1.47553028	0.60813069
H	4.45972733	-1.56313327	-1.66372781	H	2.70867313	-2.48056815	-0.77276418
H	3.04882147	-1.02000097	-2.56742497	H	3.04432051	-3.25916808	0.77841682
H	3.04772477	1.02592779	-2.56592637	H	0.88983644	-3.53377280	-0.99087172
H	4.45865038	1.56857385	-1.66193817	H	0.65378395	-4.30091717	0.57187830
H	2.99288349	2.57042660	0.07986471	H	-1.47334380	-3.04734597	0.91575700
H	2.77310084	3.27921832	-1.53110092	H	-1.45343425	-4.16845309	-0.45701280
H	-0.55142960	1.56761176	1.88333003	H	0.98987397	-0.74076777	-1.66778069
H	-1.86944633	2.69596400	2.35949447	H	1.22554677	0.23745659	-3.16165965
H	-2.21527034	1.00365404	1.88943752	H	1.01526399	0.99393705	-1.53725362
H	-4.12901918	0.00203671	-2.48342554	H	-3.57280059	2.96767469	-0.77094095

H	-2.59921373	0.88363888	-2.19193378	H	-3.34228675	1.25648571	-1.24463286
H	-2.59898066	-0.87977606	-2.19380962	H	-3.36963031	1.67354921	0.47262314
H	-2.21530340	-1.00786285	1.88738983	H	1.36034779	0.53077666	2.12499846
H	-1.86862422	-2.70089187	2.35421756	H	1.17243034	2.10862640	2.96055988
H	-0.55116166	-1.57090604	1.88040214	H	-0.22672566	1.26555873	2.21147652
H	0.90996083	3.00724128	1.05980817	H	-0.03890588	-2.50947354	-2.34039406
H	1.04311632	4.14255730	-0.29525735	H	-1.64915535	-3.03476537	-2.83374214
H	-1.17165934	3.69966020	-1.09409108	H	-2.34229755	-0.74701147	-3.28834340
H	-1.13341713	4.26673093	0.57586580	H	-0.79037277	-1.04079473	-4.08581014
H	-3.59259998	3.27982906	0.43302676	H	-0.70552948	1.80004518	-3.78459599
H	-3.10602782	2.76434442	-1.18555737	H	-2.29344141	1.37007743	-3.13731692
H	-4.97731860	1.44817937	-0.44834874	H	-1.59127748	3.50814750	-2.19342288
H	-4.22104087	1.06180909	1.09984105	H	-0.02475018	2.83959659	-1.71802494
H	-4.22079114	-1.06550746	1.09750866	H	-1.68554371	4.11965658	0.39002835
H	-4.97668105	-1.44898105	-0.45158370	H	-1.62706037	2.72836475	1.48676698
H	-3.10464269	-2.76277324	-1.19125407	H	0.43166088	4.03231665	1.56309326
H	-3.59124344	-3.28185190	0.42617984	H	0.66595973	3.92360725	-0.17731460
Li	1.30633607	0.00054429	0.19821850	Li	-0.99968983	0.00456062	-0.13466538
Ca	1.82359675	-0.00619658	3.99193317	Ca	-2.88391324	-0.36609464	3.68523415

Chair (Na-HMHC)-Be				Boat (Na-HMHC)-Be			
N	1.30080669	-2.39573574	-0.37414079	N	-2.75296203	-0.43171361	-0.89453352
N	3.18331698	-0.00046971	0.06825394	N	-1.62128137	2.05995446	0.54419892
N	1.30159006	2.39540444	-0.37408095	N	1.39751651	2.43904626	0.32737989
N	-1.60598455	2.38831647	0.42305944	N	1.81905439	0.24685455	-1.52359438
N	-2.89497768	0.00036739	-0.58836648	N	2.08212810	-1.91738081	0.37260499
N	-1.60675732	-2.38784323	0.42311809	N	-0.93359844	-2.43853930	0.58976880
C	0.95374513	-2.57890681	-1.77062362	C	-2.68978516	-0.45782645	-2.33923323
C	3.84285922	-0.00057752	1.36664506	C	-2.02579578	1.79856723	1.91673842
C	0.95461508	2.57873196	-1.77055970	C	2.66293727	2.40148827	1.03896638
C	-0.81220432	-3.59576052	0.28989166	C	-2.05154348	-2.75415734	-0.28886077
C	0.67889152	-3.38949248	0.50398197	C	-3.16183686	-1.71104243	-0.34542252
C	2.74549556	-2.43392230	-0.16849607	C	-3.52003882	0.70010569	-0.40709217
C	3.49095032	-1.20978881	-0.67819290	C	-2.74876491	2.01444181	-0.37650138
C	3.49133933	1.20876743	-0.67816157	C	-0.94424425	3.34665327	0.43523265
C	2.74628830	2.43311981	-0.16840981	C	0.48401014	3.37565693	0.96600215
C	-1.82573639	2.03844904	1.81507516	C	0.51152205	0.00508549	-2.08834055
C	-2.22001630	0.00018729	-1.86274056	C	3.23418368	-1.47287827	1.13760386
C	-1.82635967	-2.03784993	1.81512454	C	-1.34939332	-2.28941797	1.97574087
C	0.67994036	3.38933477	0.50402131	C	1.56986296	2.67852796	-1.09349199
C	-0.81107796	3.59600472	0.28980894	C	2.33672850	1.56836058	-1.81181506
C	-2.83839581	2.48004711	-0.33571343	C	2.75992052	-0.82707823	-1.76346035
C	-3.66504155	1.19840981	-0.33575147	C	2.39153395	-2.11763900	-1.03073694
C	-3.66545789	-1.19738481	-0.33567035	C	1.46967490	-3.07666668	1.00300917
C	-2.83922625	-2.47927599	-0.33558822	C	0.09849981	-3.45905242	0.45840286
H	-0.12307639	-2.43254598	-1.92311272	H	-2.02005701	-1.25426360	-2.69171848
H	1.22532323	-3.58875293	-2.14980473	H	-3.68954176	-0.62805712	-2.79846867

H	1.46976786	-1.83750595	-2.39574592	H	-2.29857689	0.49014388	-2.73346772
H	4.94940504	-0.00075019	1.25771848	H	-2.84126361	2.47905356	2.24693795
H	3.54068714	-0.87496867	1.95795446	H	-1.17447489	1.91554621	2.60090533
H	3.54096206	0.87390873	1.95795566	H	-2.36564157	0.76158718	2.03767670
H	1.47039564	1.83716938	-2.39569110	H	3.21486269	3.36383135	0.96492004
H	1.22654547	3.58849532	-2.14970711	H	3.30621912	1.60425444	0.64476062
H	-0.12225568	2.43275146	-1.92306314	H	2.48379641	2.17574724	2.10076713
H	-0.98463791	-4.01878747	-0.71150070	H	-2.52332769	-3.71974059	0.00684458
H	-1.14564016	-4.38120507	1.00281442	H	-1.65178116	-2.91170795	-1.30371767
H	0.87667302	-3.07535036	1.54357932	H	-4.00064069	-2.15440802	-0.92744108
H	1.16307526	-4.38230053	0.36722169	H	-3.55986909	-1.54996715	0.66571500
H	3.18271286	-3.33820992	-0.64719498	H	-3.88499004	0.47247869	0.60378427
H	2.92308197	-2.54132005	0.91130798	H	-4.43283779	0.86642516	-1.02118967
H	4.58014811	-1.43386123	-0.65232872	H	-2.37291553	2.23938795	-1.38809421
H	3.24573546	-1.03962405	-1.73733107	H	-3.48359091	2.81745268	-0.13583328
H	3.24606022	1.03871844	-1.73730504	H	-0.95351847	3.64872641	-0.62265716
H	4.58060866	1.43248979	-0.65229405	H	-1.51260538	4.13923453	0.97034900
H	2.92391028	2.54040984	0.91139971	H	0.48615977	3.14787122	2.04359716
H	3.18380454	3.33728263	-0.64707039	H	0.85007880	4.42313545	0.87106283
H	-0.86905618	1.97139180	2.35859497	H	-0.19304888	0.78459386	-1.76758420
H	-2.47081910	2.78044953	2.33587687	H	0.51919954	-0.02781006	-3.20071950
H	-2.29937393	1.05163120	1.89121081	H	0.10007620	-0.94267155	-1.71353394
H	-2.92101666	0.00027126	-2.72844962	H	4.03883686	-2.23957211	1.16875746
H	-1.57264097	0.88235485	-1.94742711	H	3.65306327	-0.55407256	0.70785968
H	-1.57293604	-0.88220881	-1.94735754	H	2.91734980	-1.22952778	2.16350759
H	-2.29968492	-1.05088000	1.89123768	H	-2.07044619	-1.46899824	2.08116950
H	-2.47166341	-2.77962956	2.33596758	H	-1.81477733	-3.21844337	2.37354189
H	-0.86964340	-1.97108173	2.35861702	H	-0.49441632	-2.00803409	2.60805621
H	0.87756275	3.07514091	1.54363309	H	0.57940397	2.78099105	-1.55696413
H	1.16441647	4.38200287	0.36728173	H	2.09924296	3.63931608	-1.28705618
H	-0.98331179	4.01901094	-0.71162928	H	3.39340576	1.59392661	-1.50816935
H	-1.14433312	4.38159291	1.00265740	H	2.32660230	1.79558067	-2.90144734
H	-3.49758649	3.29537090	0.04208212	H	2.86006302	-1.06587531	-2.84632154
H	-2.58308979	2.75631748	-1.37203735	H	3.75336062	-0.48726810	-1.43571212
H	-4.48833123	1.33151368	-1.07598640	H	3.22767684	-2.84007171	-1.16862627
H	-4.15656778	1.08015901	0.64261564	H	1.52042895	-2.56924495	-1.52423977
H	-4.15691732	-1.07891319	0.64270363	H	2.12317840	-3.97441921	0.91804586
H	-4.48880470	-1.33026238	-1.07588223	H	1.39048598	-2.85353900	2.07790353
H	-2.58404275	-2.75568398	-1.37190637	H	-0.20946183	-4.39863906	0.96997051
H	-3.49865244	-3.29437311	0.04228673	H	0.18227831	-3.72219857	-0.60677722
Na	0.48529423	-0.00003772	0.45381993	Na	0.42967727	0.05574521	0.78445377
Be	1.09133956	-0.00015922	3.42083522	Be	0.92368399	0.50493179	3.86334843

Chair (Na-HMHC)-Mg				Boat (Na-HMHC)-Mg			
N	-1.13310308	2.52018418	-0.48897104	N	2.87951509	-0.46952642	-0.76963535
N	-3.12725722	0.18030101	-0.24306802	N	0.83185619	-2.48932439	0.37396853
N	-1.30953609	-2.25898016	-0.68782605	N	-2.08681849	-1.80417833	-0.14885852

N	1.57699711	-2.46459918	0.18724401	N	-1.53486134	0.47941707	-1.86608122
N	2.96918221	-0.03114800	-0.57366204	N	-1.29223646	2.51831571	0.17795841
N	1.70961412	2.35239617	0.51418804	N	1.67749841	1.97212595	0.69811496
C	-0.67059005	2.75238720	-1.84370913	C	3.00192557	-0.36954112	-2.20782610
C	-3.83588628	0.20568201	1.02736807	C	1.14716139	-2.44616882	1.79328370
C	-0.92061907	-2.29719916	-2.08416615	C	-3.35062731	-1.37845286	0.42708277
C	0.96927507	3.59500426	0.39427003	C	2.92339072	1.92659366	-0.05603553
C	-0.54215204	3.44011625	0.48307503	C	3.62507630	0.57399177	-0.08970776
C	-2.58735719	2.60196219	-0.40001603	C	3.16647709	-1.81184197	-0.29607864
C	-3.32796124	1.41009810	-0.98989007	C	2.00485717	-2.78821397	-0.43682051
C	-3.46795425	-1.00707807	-1.01012207	C	-0.21818464	-3.46567307	0.10544662
C	-2.75987720	-2.26352416	-0.52374304	C	-1.62439128	-3.02672928	0.49457183
C	1.76746313	-2.27201516	1.61192311	C	-0.17408713	0.30077148	-2.31867700
C	2.36619517	0.09463601	-1.87774713	C	-2.60655426	2.46829791	0.79528763
C	1.82190813	1.91523814	1.89330014	C	1.87205485	1.63125028	2.09899264
C	-0.75236306	-3.36704424	0.08958001	C	-2.15055185	-1.90905063	-1.59611337
C	0.73769105	-3.61395126	-0.09770401	C	-2.42612945	-0.57915809	-2.29564230
C	2.83120320	-2.52191018	-0.53742904	C	-2.04586754	1.81591771	-2.09188456
C	3.69119226	-1.27107509	-0.38703803	C	-1.35575955	2.87153511	-1.22855234
C	3.76417127	1.11392208	-0.18714501	C	-0.40234064	3.37424788	0.94863127
C	2.99294322	2.42976118	-0.15729601	C	1.06886927	3.28991421	0.56046894
H	0.40875703	2.57238919	-1.92001314	H	2.68319060	0.61965495	-2.56415825
H	-0.87723707	3.78760627	-2.19439816	H	4.04855550	-0.53162924	-2.55014514
H	-1.16143008	2.05938215	-2.54032018	H	2.36792369	-1.11299123	-2.71027330
H	-4.92583136	0.37030003	0.88060107	H	1.64981827	-3.37627796	2.13753579
H	-3.43681125	0.98647207	1.68840912	H	0.23318041	-2.30776344	2.38705933
H	-3.69938627	-0.73940106	1.56888611	H	1.79352331	-1.59102079	2.03068377
H	-1.35528010	-1.44805710	-2.62869219	H	-4.17565897	-2.08814021	0.20117302
H	-1.24405809	-3.23077923	-2.59549319	H	-3.63520630	-0.38647685	0.05333890
H	0.16881301	-2.21186016	-2.18022016	H	-3.24958864	-1.29373295	1.51935031
H	1.22986309	4.06593329	-0.56555704	H	3.65333825	2.66507924	0.34847923
H	1.27480009	4.32752631	1.17321908	H	2.70808092	2.24814482	-1.08796487
H	-0.82827006	3.08282522	1.48683311	H	4.62238497	0.73140780	-0.55751348
H	-0.97494707	4.45922932	0.36876503	H	3.83220182	0.24751208	0.93848600
H	-2.95656921	3.52658525	-0.89619606	H	3.46760794	-1.75924484	0.75910808
H	-2.85433721	2.70080820	0.66174405	H	4.03656987	-2.25301414	-0.83064852
H	-4.40727732	1.67472412	-1.05116407	H	1.68899083	-2.82864156	-1.49207590
H	-2.99837222	1.24669709	-2.02700714	H	2.39943001	-3.80191169	-0.19444686
H	-3.22206623	-0.82604606	-2.06678715	H	-0.18928814	-3.71269705	-0.96613649
H	-4.56199033	-1.20315209	-0.98762507	H	-0.01215136	-4.42320995	0.63195283
H	-2.97158322	-2.40924317	0.54648104	H	-1.67755048	-2.86422970	1.58316760
H	-3.20782623	-3.13736322	-1.04787407	H	-2.30830654	-3.87813665	0.27865582
H	0.79996406	-2.26896116	2.13319815	H	0.20428160	-0.68394383	-2.01228302
H	2.40041117	-3.06892522	2.06143515	H	-0.06976771	0.39032113	-3.42282653
H	2.22968216	-1.29713309	1.81294613	H	0.48856423	1.03805791	-1.84435425
H	3.11448022	0.14466801	-2.70142320	H	-3.10433578	3.46247590	0.80353021
H	1.70181912	-0.75671505	-2.07131215	H	-3.25846584	1.76339704	0.26362723
H	1.74682413	0.99878607	-1.92167414	H	-2.50930114	2.09826835	1.82841325

H	2.25150316	0.90655907	1.94161014	H	2.25159323	0.60687269	2.20391214
H	2.45257918	2.60189319	2.50126518	H	2.58495340	2.32195343	2.60171937
H	0.82854206	1.84119613	2.36183217	H	0.91284630	1.64477429	2.63865979
H	-0.97719907	-3.17271723	1.15174908	H	-1.19607896	-2.30962254	-1.96306136
H	-1.26753809	-4.31904731	-0.16901001	H	-2.93195787	-2.63367898	-1.91944550
H	0.92623907	-3.93581028	-1.13301108	H	-3.45845214	-0.26104960	-2.09046000
H	1.01071007	-4.48597032	0.53572104	H	-2.37282733	-0.75254660	-3.39353306
H	3.45517325	-3.38842124	-0.21806202	H	-1.95021179	2.12837927	-3.15596404
H	2.60559619	-2.69142120	-1.60287911	H	-3.12389048	1.80861050	-1.87448274
H	4.54624632	-1.36711810	-1.09636808	H	-1.88295424	3.83964052	-1.38463201
H	4.13728430	-1.25193009	0.61967805	H	-0.33414487	3.02267326	-1.60220384
H	4.18239230	0.91026206	0.81121306	H	-0.70574093	4.44293661	0.87300235
H	4.64142734	1.26052209	-0.86000406	H	-0.52283141	3.09302453	2.00644509
H	2.81880320	2.77847720	-1.18841608	H	1.61586648	4.04136759	1.17268917
H	3.66030226	3.18932523	0.31113602	H	1.19792718	3.61593227	-0.48247627
Na	-0.45212803	0.06095300	0.36914103	Na	-0.42691334	0.08456341	0.54261511
Mg	-1.41297910	-0.89247706	3.63415226	Mg	-1.59438810	-0.51872254	3.99770820

Chair (Na-HMHC)-Ca				Boat (Na-HMHC)-Ca			
N	1.13858608	-2.33540717	-0.90355107	N	3.12186733	-0.13423061	0.07988744
N	3.09847622	0.00173100	-0.70224105	N	1.04017479	-2.34907774	0.61443393
N	1.13678608	2.33750917	-0.90112107	N	-1.59518952	-2.08420299	-0.89016607
N	-1.66264312	2.40635517	0.23091202	N	-0.74146956	0.17880156	-2.49422466
N	-3.13788823	-0.00063200	-0.49399104	N	-1.42179143	2.31220810	-0.65424319
N	-1.66088912	-2.40728217	0.22853202	N	1.22683381	2.18034176	0.87001365
C	0.58479004	-2.30282416	-2.24322916	C	3.71039963	-0.08000417	-1.24069752
C	3.87802728	0.00152400	0.52607704	C	0.81947565	-2.19230523	2.04314723
C	0.58287804	2.30535517	-2.24075816	C	-3.01412209	-1.79591355	-0.76794379
C	-0.90657406	-3.59607726	-0.11673101	C	2.64987075	2.27191658	0.56785403
C	0.60653804	-3.42653525	-0.08747701	C	3.47297471	1.02694812	0.87700885
C	2.59462119	-2.42702018	-0.90967006	C	3.37657921	-1.40557779	0.73265065
C	3.31777324	-1.21097009	-1.47231411	C	2.44951700	-2.53262586	0.29302606
C	3.31676424	1.21530609	-1.47122211	C	0.26438606	-3.46470789	0.08581629
C	2.59273618	2.43026918	-0.90737306	C	-1.23295883	-3.21191097	-0.04333089
C	-1.60233912	2.10717115	1.64796612	C	0.70188947	0.12888979	-2.44006063
C	-2.77906120	0.00024100	-1.89055713	C	-2.85902177	2.13080066	-0.53884785
C	-1.60121412	-2.10974415	1.64596012	C	0.98301657	1.91455306	2.27907538
C	0.60397904	3.42767025	-0.08426901	C	-1.18211241	-2.25262460	-2.27248361
C	-0.90927406	3.59607126	-0.11320901	C	-1.33495250	-0.98753234	-3.11520893
C	-3.02397122	2.48049018	-0.26432802	C	-1.25625398	1.44064786	-2.98450666
C	-3.82987527	1.19840109	-0.07547301	C	-1.01089361	2.59821270	-2.01770926
C	-3.82899027	-1.20065509	-0.07685801	C	-0.95780660	3.30414720	0.30554605
C	-3.02205422	-2.48188818	-0.26710002	C	0.55608709	3.40459988	0.44726234
H	-0.50113604	-2.15681815	-2.19853316	H	3.43165100	0.84724730	-1.75987783
H	0.79410706	-3.23085323	-2.81945420	H	4.82190442	-0.12605931	-1.20486008
H	0.99719307	-1.45581711	-2.80817720	H	3.36181965	-0.91576415	-1.86290985
H	4.96994336	0.00248500	0.31407602	H	1.21039398	-3.05478818	2.62627861

H	3.63243126	-0.87167606	1.14433308	H	-0.25351185	-2.07728399	2.25683786
H	3.63108426	0.87355407	1.14550308	H	1.29557911	-1.27678816	2.41773581
H	0.99544507	1.45868010	-2.80612020	H	-3.64652827	-2.63149602	-1.13866891
H	0.79184606	3.23368623	-2.81660320	H	-3.27570757	-0.89032494	-1.33028828
H	-0.50299004	2.15902716	-2.19601916	H	-3.25642979	-1.59573384	0.28755259
H	-1.21467009	-3.91932928	-1.12292308	H	3.11403305	3.11826624	1.12442996
H	-1.15326708	-4.44822032	0.55577604	H	2.75467672	2.51844417	-0.50125535
H	0.95339007	-3.26110023	0.94597107	H	4.54388023	1.29985684	0.74798297
H	1.03726007	-4.40019831	-0.41180903	H	3.36232796	0.77325107	1.94009911
H	2.92726521	-3.31969524	-1.48558111	H	3.29045146	-1.27024143	1.81945766
H	2.91892721	-2.59452819	0.12845001	H	4.42018834	-1.74960546	0.55916602
H	4.39913631	-1.46222310	-1.53593611	H	2.53447672	-2.66941232	-0.79742564
H	2.99319122	-1.03332007	-2.50807318	H	2.83676745	-3.47163857	0.75135352
H	2.99218221	1.03836808	-2.50713418	H	0.68156490	-3.73474040	-0.89571604
H	4.39793032	1.46741611	-1.53477211	H	0.39387315	-4.37087307	0.71813447
H	2.91707321	2.59710819	0.13084501	H	-1.66558711	-3.02051717	0.95135812
H	2.92460921	3.32373124	-1.48256211	H	-1.69812847	-4.15532960	-0.40806496
H	-0.55827104	2.03944415	1.98917114	H	1.03418116	-0.79138689	-1.94051241
H	-2.12334215	2.87332721	2.26440816	H	1.17479638	0.17526997	-3.44611648
H	-2.05165715	1.12700308	1.85392214	H	1.09177085	0.95737216	-1.83258226
H	-3.66514327	0.00010600	-2.56600618	H	-3.42106421	3.05374849	-0.79952718
H	-2.16966215	0.88124706	-2.12632015	H	-3.20160411	1.32205449	-1.19708814
H	-2.16875616	-0.87992406	-2.12715116	H	-3.10812268	1.83065334	0.49110978
H	-2.05134715	-1.13017308	1.85297614	H	1.39580993	0.94136183	2.57417395
H	-2.12177615	-2.87704821	2.26134116	H	1.42515613	2.69571497	2.93582375
H	-0.55728604	-2.04158115	1.98751614	H	-0.09697297	1.85140714	2.47916586
H	0.95109407	3.26181724	0.94902007	H	-0.12925978	-2.56451142	-2.28996484
H	1.03389907	4.40190132	-0.40796803	H	-1.75118191	-3.06830049	-2.77291720
H	-1.21770009	3.92007028	-1.11906008	H	-2.40235679	-0.78008908	-3.27934391
H	-1.15656708	4.44736632	0.56015504	H	-0.90555767	-1.19253043	-4.12126741
H	-3.59613726	3.30243724	0.22472702	H	-0.81951057	1.71866438	-3.96968271
H	-2.98486722	2.73894320	-1.33502210	H	-2.33655777	1.32451743	-3.15465405
H	-4.79720534	1.33371010	-0.61397805	H	-1.52889601	3.49742105	-2.42070874
H	-4.09246230	1.08276308	0.98778607	H	0.05997848	2.84125623	-2.02076844
H	-4.09177729	-1.08641708	0.98650207	H	-1.33522432	4.31967614	0.04916109
H	-4.79616135	-1.33609910	-0.61561705	H	-1.40618065	3.04627477	1.27789347
H	-2.98251421	-2.73898420	-1.33810310	H	0.76755996	4.23457173	1.15738201
H	-3.59366426	-3.30489124	0.22082002	H	0.99834280	3.72176176	-0.50881548
Na	0.56265304	0.00004300	0.21889902	Na	-0.50492358	0.02182610	0.17376423
Ca	1.49328311	-0.00362000	4.28826831	Ca	-2.82190330	-0.17167125	3.93165094

Chair (K-HMHC)-Be				Boat (K-HMHC)-Be			
N	0.02466869	-2.78537962	-0.44918676	N	-0.13563500	2.58026800	-0.95708100
N	2.66294863	-1.45454672	0.19312278	N	2.50750100	1.51213100	0.27732100
N	2.41218091	1.46706393	-0.44786334	N	2.48975600	-1.56900100	0.44842500
N	-0.02935722	2.99950399	0.37352385	N	0.12536700	-2.27843100	-1.17189100
N	-2.43835288	1.42051087	-0.45317386	N	-2.33780300	-1.77332500	0.39840300

N	-2.63519768	-1.50174102	0.19990797	N	-2.64387000	1.29018600	0.32730500
C	0.01667422	-2.47727340	-1.86202216	C	-0.18890800	2.28674500	-2.37546500
C	2.84719818	-1.45977408	1.63555338	C	2.64748200	2.01648500	1.63531400
C	2.02094775	1.37168925	-1.83754160	C	2.23267000	-2.45872700	1.56669800
C	-2.49253492	-2.84886558	-0.32687980	C	-2.62178900	2.44216000	-0.56017700
C	-1.15774199	-3.51602985	-0.01174721	C	-1.33985600	3.26667800	-0.50317700
C	1.22295783	-3.49535228	-0.02123304	C	1.05293200	3.35449700	-0.61808800
C	2.54327518	-2.80142259	-0.33982542	C	2.37066700	2.58946900	-0.68985500
C	3.69880845	-0.69431617	-0.48039372	C	3.59622300	0.61655400	-0.08452700
C	3.67793713	0.80090255	-0.18039585	C	3.62979500	-0.69726200	0.69160500
C	-0.03713237	2.94271389	1.82600696	C	0.10718400	-1.16383600	-2.09136800
C	-2.04285527	1.32099103	-1.84135739	C	-2.01859500	-2.66507400	1.49865700
C	-2.81528351	-1.50331807	1.64283450	C	-2.81608200	1.68587900	1.71715100
C	2.45401221	2.83595403	0.04466099	C	2.60380900	-2.26865000	-0.81710100
C	1.16886890	3.63617854	-0.14382896	C	1.35577800	-3.04428200	-1.23199500
C	-1.23362697	3.61252603	-0.15794900	C	-1.04915700	-3.12276000	-1.28133800
C	-2.50692552	2.79268617	0.02670718	C	-2.35895700	-2.44378800	-0.88864700
C	-3.69193954	0.73317213	-0.18203528	C	-3.56419600	-1.02514000	0.63499500
C	-3.68626805	-0.76363195	-0.47458702	C	-3.63804600	0.31469800	-0.09221700
H	-0.87144822	-1.88361572	-2.11899545	H	-1.04168800	1.63769700	-2.61262500
H	0.02217091	-3.38406546	-2.50770777	H	-0.28051400	3.20970000	-2.99069000
H	0.89228856	-1.86816945	-2.12581661	H	0.71523300	1.75529000	-2.69928000
H	3.83438164	-1.88176197	1.92474781	H	3.59306600	2.58547800	1.77136500
H	2.06493381	-2.05017410	2.13393744	H	2.61738100	1.19874600	2.36802400
H	2.76625961	-0.44552396	2.05086157	H	1.80998500	2.67300300	1.90413400
H	1.92282721	0.31879609	-2.13537026	H	3.05235000	-3.19239400	1.72968200
H	2.74724525	1.85751376	-2.52686217	H	1.30079900	-3.01775700	1.40570500
H	1.04047255	1.83911085	-1.99153514	H	2.08924600	-1.87242500	2.48748000
H	-2.63613897	-2.81023526	-1.41766720	H	-3.46836700	3.13134300	-0.34330700
H	-3.29290139	-3.52114587	0.05452168	H	-2.78721800	2.08983800	-1.58925200
H	-1.06377920	-3.67396271	1.07430125	H	-1.51304000	4.19325700	-1.09676800
H	-1.18900447	-4.53108794	-0.47083985	H	-1.16918100	3.59843700	0.53140000
H	1.27101211	-4.50761258	-0.48503429	H	0.92042100	3.75210200	0.39800500
H	1.13762841	-3.66004527	1.06447524	H	1.14572700	4.24466200	-1.28056800
H	3.35820892	-3.46030093	0.03415279	H	2.49295500	2.16330800	-1.69738900
H	2.68059271	-2.75453093	-1.43110988	H	3.19112800	3.33431200	-0.57823400
H	3.59851472	-0.85513324	-1.56513782	H	3.51570600	0.40144200	-1.16183700
H	4.71559708	-1.06413308	-0.21481081	H	4.58391100	1.11329400	0.05309100
H	3.92824092	0.96898326	0.87793929	H	3.67173900	-0.48306100	1.76831500
H	4.50423613	1.26505132	-0.76664962	H	4.58713500	-1.21024500	0.45112600
H	0.83951329	2.40299130	2.21025292	H	0.95733300	-0.49330000	-1.89937800
H	-0.05058932	3.95646590	2.28294023	H	0.15184100	-1.48091500	-3.15721100
H	-0.90675322	2.38470965	2.19976856	H	-0.80653600	-0.56953900	-1.95211000
H	-2.77680442	1.78775098	-2.53573068	H	-2.76091700	-3.48431000	1.61912200
H	-1.07094738	1.80525030	-1.99763588	H	-1.02894600	-3.11830000	1.35020900
H	-1.92474867	0.26777608	-2.13045845	H	-1.96240200	-2.09496200	2.43840900
H	-2.75202656	-0.48574197	2.05308071	H	-2.08143300	2.44962400	2.00336900
H	-3.79372029	-1.94194324	1.93692395	H	-3.83196600	2.09471700	1.90955500

H	-2.02091314	-2.07699254	2.14170814	H	-2.63754600	0.84342800	2.40001300
H	2.71688618	2.79639801	1.11329937	H	2.85663400	-1.53773900	-1.59960600
H	3.26698260	3.41631688	-0.44972023	H	3.44890500	-2.99540000	-0.80232000
H	1.01711496	3.83212249	-1.21641915	H	1.23757900	-3.92076200	-0.57710100
H	1.33491394	4.63425797	0.32075956	H	1.53977500	-3.45050500	-2.25300800
H	-1.41999893	4.61111564	0.29794501	H	-1.17674900	-3.52048500	-2.31413400
H	-1.07640181	3.80296874	-1.23079681	H	-0.89036300	-4.00250900	-0.63991600
H	-3.32532268	3.35508913	-0.47938255	H	-3.15127800	-3.22730400	-0.92103800
H	-2.77817017	2.75832511	1.09337537	H	-2.63799900	-1.70983200	-1.65940700
H	-3.94501810	0.90212809	0.87552529	H	-4.45923900	-1.61858900	0.34521200
H	-4.52656458	1.17933912	-0.77048635	H	-3.65971700	-0.85601300	1.71625300
H	-3.58568376	-0.92784910	-1.55879496	H	-4.67058300	0.71108700	0.04492800
H	-4.69558898	-1.15045126	-0.20477434	H	-3.51808800	0.14995400	-1.17497100
K	0.00377238	-0.04042143	0.59445389	K	-0.00051500	0.02516400	0.81107700
Be	0.01859104	-1.09470870	3.87162057	Be	0.00544200	0.90320700	4.14353400

Chair (K-HMHC)-Mg				Boat (K-HMHC)-Mg			
N	1.32087828	2.53798488	-0.50162169	N	0.21065857	-2.67948532	-0.95770017
N	-1.64846619	2.51041281	-0.05938965	N	-2.49456251	-1.48032506	0.04642726
N	-2.68017353	-0.22366397	-0.79592574	N	-2.41146774	1.60123448	-0.06583560
N	-1.21507969	-2.74473071	-0.04765634	N	0.12573168	2.09148125	-1.52155988
N	1.71452492	-2.29368748	-0.50106521	N	2.38727565	1.74592292	0.34508686
N	3.03060845	0.24381166	0.38583900	N	2.61604099	-1.32879525	0.47387749
C	1.32951809	2.16117294	-1.89881997	C	0.35786491	-2.51953065	-2.39146277
C	-1.78301079	2.65615230	1.38049240	C	-2.73217375	-1.90378306	1.41793716
C	-2.24485017	-0.19662633	-2.17529860	C	-2.28174238	2.68211529	0.89610662
C	3.57873714	1.49723939	-0.10144907	C	2.65605778	-2.51466080	-0.36748468
C	2.65627297	2.70197798	0.05476906	C	1.37277484	-3.33990070	-0.37492936
C	0.52760984	3.73221587	-0.25029420	C	-1.01512859	-3.39887736	-0.62922164
C	-0.94026703	3.63082304	-0.65104242	C	-2.30648108	-2.61551433	-0.84370381
C	-2.93329747	2.28158430	-0.70010446	C	-3.55546899	-0.60451419	-0.43515202
C	-3.53450340	0.90335570	-0.44440936	C	-3.58652926	0.78275450	0.20092130
C	-1.31103464	-2.89390986	1.39477390	C	0.27656028	0.88977271	-2.30943519
C	1.64733419	-1.91871053	-1.89711593	C	1.99255091	2.72878395	1.33858907
C	2.91114961	0.22533577	1.83426066	C	2.64023923	-1.66650982	1.88878841
C	-3.33976871	-1.47000905	-0.42805901	C	-2.37574938	2.07616048	-1.43704744
C	-2.52569184	-2.73555411	-0.67656810	C	-1.09617227	2.81451772	-1.82180328
C	-0.33882570	-3.74044270	-0.63664668	C	1.29569273	2.94783925	-1.56535761
C	1.12829471	-3.60091467	-0.24500039	C	2.55704614	2.32072533	-0.97650728
C	3.06495502	-2.23973170	0.03970023	C	3.55627385	0.98517750	0.76189109
C	3.77416846	-0.89827325	-0.11548417	C	3.67470511	-0.39431721	0.11950443
H	1.89206408	1.22961104	-2.03971911	H	1.24196181	-1.91588031	-2.63340201
H	1.77992075	2.93881414	-2.55513840	H	0.45978721	-3.49815754	-2.91111054
H	0.30612610	1.97193366	-2.25013511	H	-0.50941073	-2.00120542	-2.82006842
H	-2.32544431	3.58621462	1.65649090	H	-3.64284154	-2.53534600	1.50553510
H	-0.80080280	2.66846860	1.87460306	H	-2.85211602	-1.03931910	2.08602673
H	-2.33329686	1.80819293	1.81361835	H	-1.87869946	-2.47222253	1.81195779

H	-1.69702439	0.73216843	-2.38538413	H	-3.06676478	3.45960973	0.77319018
H	-3.08659445	-0.26997339	-2.89965722	H	-1.29945011	3.16662140	0.80396887
H	-1.55287002	-1.02620418	-2.37430379	H	-2.35245078	2.28530351	1.92040923
H	3.83469287	1.36969964	-1.16455612	H	3.48456582	-3.19339066	-0.06344893
H	4.53583769	1.75052980	0.40746792	H	2.89470765	-2.20010920	-1.39456430
H	2.54323434	2.95097130	1.12152846	H	1.59238265	-4.29411999	-0.90548717
H	3.18003428	3.56933793	-0.40891933	H	1.11960655	-3.62270060	0.65705498
H	0.95214986	4.61264922	-0.78523841	H	-0.95457481	-3.71416165	0.42212188
H	0.60479351	3.96541709	0.82264141	H	-1.09117177	-4.33848731	-1.22149835
H	-1.41795193	4.60134240	-0.38623145	H	-2.34278560	-2.24842431	-1.88055894
H	-1.01851519	3.55075516	-1.74635062	H	-3.14925159	-3.33774320	-0.75078294
H	-2.80915022	2.43351175	-1.78327939	H	-3.44383859	-0.50639485	-1.52590480
H	-3.68803194	3.03308221	-0.37853858	H	-4.55562902	-1.06640984	-0.27585128
H	-3.79984286	0.79840301	0.61955957	H	-3.69010382	0.68627238	1.29193151
H	-4.49630916	0.86279753	-1.00543270	H	-4.51595966	1.28827433	-0.14445286
H	-1.99352171	-2.14590479	1.82397979	H	-0.59965614	0.23832180	-2.18435796
H	-1.68676553	-3.89854000	1.68627449	H	0.39867032	1.09643146	-3.39619680
H	-0.33666764	-2.73513056	1.87898817	H	1.15088802	0.31585153	-1.97084191
H	2.20992461	-2.61313948	-2.56018661	H	2.74954761	3.53222577	1.47239107
H	0.60318643	-1.89604167	-2.23704978	H	1.04049160	3.19931883	1.05691532
H	2.05195975	-0.90890502	-2.04076030	H	1.82418224	2.23432202	2.30830531
H	2.41632884	-0.69166868	2.18437165	H	1.85556257	-2.39529911	2.12994016
H	3.90023629	0.29894940	2.33711137	H	3.61858403	-2.09630468	2.19791362
H	2.28118423	1.05072578	2.19537323	H	2.42209986	-0.79037044	2.51732819
H	-3.61138788	-1.39880528	0.63723739	H	-2.51938389	1.22021431	-2.11228203
H	-4.29904113	-1.59048183	-0.98186500	H	-3.22507651	2.76778992	-1.64396426
H	-2.38858464	-2.87820767	-1.75945618	H	-1.05742959	3.77658803	-1.28976539
H	-3.14542089	-3.59565340	-0.33910171	H	-1.16853034	3.06890195	-2.90376559
H	-0.65198006	-4.77346148	-0.36250267	H	1.53622054	3.26558604	-2.60577987
H	-0.43516834	-3.68203829	-1.73194369	H	1.05655928	3.87117600	-1.01662092
H	1.68700145	-4.40097147	-0.78297941	H	3.34415473	3.10965625	-0.97466640
H	1.24937781	-3.81782311	0.82731874	H	2.92596911	1.53731305	-1.65494981
H	3.00747010	-2.51149165	1.10525624	H	4.49601344	1.54038464	0.54731616
H	3.71884441	-3.00582817	-0.43699152	H	3.51953446	0.87563234	1.85482365
H	3.99544844	-0.72369528	-1.17971988	H	4.67433632	-0.80417783	0.39146696
H	4.76468748	-0.99288228	0.38380605	H	3.68046543	-0.28825576	-0.97686478
K	-0.00675483	0.00944638	0.44814686	K	-0.01092027	0.01671308	0.67598616
Mg	-1.45571477	-0.09926749	4.03512818	Mg	-1.21511153	0.51945614	4.29941525

Chair (K-HMHC)-Ca				Boat (K-HMHC)-Ca			
N	1.63414447	-2.42270571	-0.51326076	N	0.48396356	-2.80903654	-0.73280291
N	3.06374440	0.02290538	0.47378899	N	-2.37519491	-1.62954174	-0.31642167
N	1.59522729	2.44688013	-0.51151633	N	-2.37669929	1.40873665	-0.85427274
N	-1.40013653	2.60015382	-0.40949718	N	0.32996664	1.83500817	-1.96702212
N	-2.51172053	-0.01907819	-1.34097418	N	2.33268568	1.84994269	0.20429382
N	-1.36089519	-2.62060211	-0.40512661	N	2.63340410	-1.16077679	0.80068186
C	1.71334218	-2.10981276	-1.92381026	C	0.81135313	-2.83863653	-2.14514975

C	2.85171200	0.01853734	1.91236391	C	-2.82398675	-1.84139508	1.05065088
C	1.68334063	2.13101136	-1.92092201	C	-2.42121883	2.58592182	-0.00531289
C	-0.50307502	-3.72364155	-0.80138659	C	2.82234505	-2.43984510	0.13406795
C	0.91546500	-3.66002449	-0.24420553	C	1.58146079	-3.32505580	0.07702630
C	2.93810304	-2.45645281	0.13351759	C	-0.74731092	-3.54071975	-0.45797063
C	3.75285241	-1.17233995	0.02122433	C	-2.02503954	-2.88237429	-0.96837021
C	3.73337089	1.23117694	0.02644226	C	-3.35707244	-0.88838927	-1.09657284
C	2.89648568	2.50093310	0.13948367	C	-3.55050673	0.56594273	-0.67595905
C	-1.73041551	2.64728689	1.00451556	C	0.59329018	0.53242362	-2.53431137
C	-1.84373954	-0.01368962	-2.62477424	C	1.79162883	2.96019953	0.96790257
C	-1.69409160	-2.67136189	1.00824591	C	2.47664282	-1.31771895	2.23811248
C	0.85887093	3.67504706	-0.24916462	C	-2.15469135	1.73962492	-2.25016557
C	-0.55963248	3.71529046	-0.80839436	C	-0.84514697	2.47134627	-2.53137485
C	-2.58755531	2.49507304	-1.23980569	C	1.48679477	2.70967796	-1.99367522
C	-3.32874419	1.16670868	-1.12401232	C	2.66677359	2.21978409	-1.15873798
C	-3.31021039	-1.21745491	-1.12436673	C	3.45244640	1.21502099	0.88385695
C	-2.54802586	-2.53404221	-1.23815889	C	3.70525946	-0.23229358	0.47082614
H	0.70645340	-2.03049921	-2.35461102	H	1.70806467	-2.24163144	-2.35480563
H	2.27824583	-2.87088684	-2.50683110	H	0.99826671	-3.87382459	-2.50785798
H	2.20131083	-1.13729336	-2.07251620	H	-0.00181735	-2.41357536	-2.74720979
H	3.81029335	0.02536080	2.47627655	H	-3.76350807	-2.43463347	1.09372388
H	2.27113985	-0.85910536	2.22997454	H	-2.99159614	-0.88575558	1.56626354
H	2.25774896	0.88620435	2.23270473	H	-2.05939137	-2.36322177	1.64132126
H	2.18380813	1.16417718	-2.06508696	H	-3.22962479	3.29282108	-0.29291861
H	2.24067905	2.89746151	-2.50417630	H	-1.46417270	3.12458980	-0.04241482
H	0.67903029	2.03794069	-2.35491724	H	-2.57538743	2.28752379	1.04251761
H	-0.46354332	-3.75048545	-1.90113908	H	3.62817055	-3.03094045	0.62492107
H	-0.93098115	-4.70424499	-0.49439557	H	3.18025962	-2.24518317	-0.88806476
H	0.89528069	-3.80158470	0.84763453	H	1.90271602	-4.32744325	-0.28650326
H	1.46300483	-4.53841230	-0.65666848	H	1.20408762	-3.48425119	1.09745319
H	3.56823213	-3.27702312	-0.28012869	H	-0.82297452	-3.68154537	0.62984050
H	2.77679189	-2.70415012	1.19404762	H	-0.70267635	-4.56491840	-0.89266178
H	4.69956031	-1.33605897	0.58364012	H	-1.93248849	-2.69317402	-2.04833172
H	4.05409943	-1.01989261	-1.02673827	H	-2.84531391	-3.62814721	-0.86480670
H	4.04052818	1.08690803	-1.02092952	H	-3.04796301	-0.92545012	-2.15258721
H	4.67539190	1.40956526	0.59219391	H	-4.35375422	-1.38327365	-1.05568364
H	2.72766567	2.74337816	1.20010459	H	-3.83959746	0.60548337	0.38389174
H	3.51405177	3.33285071	-0.27044562	H	-4.42305422	0.96606537	-1.23853602
H	-0.82410626	2.63082423	1.62679856	H	-0.28196732	-0.12118306	-2.41321259
H	-2.31871518	3.55256052	1.26850179	H	0.84520401	0.57390587	-3.61761530
H	-2.31617260	1.76606641	1.30184874	H	1.42748510	0.04694038	-2.00842193
H	-2.55196075	-0.01809446	-3.48299578	H	2.50441199	3.80927398	1.05507621
H	-1.20260251	0.87284561	-2.71775527	H	0.86876931	3.33381178	0.50289929
H	-1.19053187	-0.89123533	-2.71881473	H	1.51931349	2.62195593	1.97967658
H	-2.29114815	-1.79720967	1.30398162	H	1.66693770	-2.02191627	2.47011031
H	-2.27196152	-3.58368170	1.27098874	H	3.40797145	-1.68769621	2.72101205
H	-0.78960818	-2.64381926	1.63278031	H	2.18214088	-0.37196516	2.71544358
H	0.83530927	3.82155317	0.84192517	H	-2.18837798	0.81308025	-2.84148969

H	1.39441399	4.55918656	-0.66506711	H	-2.97707305	2.37849052	-2.64714493
H	-0.51932459	3.73924987	-1.90821648	H	-0.90244477	3.49220002	-2.12478146
H	-1.00311321	4.69005053	-0.50479473	H	-0.75963441	2.58929069	-3.63581862
H	-3.32090908	3.29971307	-1.00863052	H	1.85756057	2.87156010	-3.03172479
H	-2.28949181	2.65813950	-2.28699059	H	1.16819290	3.69861515	-1.63107669
H	-4.17557089	1.20638966	-1.84686070	H	3.43789212	3.02410996	-1.17979970
H	-3.78825738	1.07814465	-0.12740261	H	3.12964381	1.35400870	-1.65451935
H	-3.77243191	-1.13555124	-0.12844958	H	4.39590670	1.78228611	0.72284560
H	-4.15533315	-1.27099263	-1.84831536	H	3.26201930	1.25739823	1.96549485
H	-2.24517065	-2.69265575	-2.28464825	H	4.66502656	-0.55001332	0.93853095
H	-3.26923414	-3.34997564	-1.00833554	H	3.87145326	-0.27893758	-0.61680234
K	0.04875279	-0.00139162	0.24556939	K	-0.05871097	0.07706690	0.48976862
Ca	-1.75400195	-0.01028091	4.50209960	Ca	-1.72640888	1.05997950	4.61739561

Table S1. Electronic first hyperpolarizability tensors (β_{zzz}^e , a.u.) at the ω B97XD method with different basis sets.

	chair form		boat form	
	ma-SVP	ma-TZVP	ma-SVP	ma-TZVP
$\delta^+(\text{Li-HMHC})\text{-AM}^{\delta-}$				
AM ⁺ = Be	1.02×10^4	1.07×10^4	1.15×10^4	1.26×10^4
AM ⁺ = Mg	2.33×10^4	2.39×10^4	2.78×10^4	2.95×10^4
AM ⁺ = Ca	1.96×10^4	2.57×10^4	1.86×10^4	3.10×10^4
$\delta^+(\text{Na-HMHC})\text{-AM}^{\delta-}$				
AM ⁺ = Be	1.21×10^4	1.59×10^4	1.44×10^4	1.81×10^4
AM ⁺ = Mg	2.69×10^4	2.67×10^4	3.44×10^4	3.47×10^4
AM ⁺ = Ca	2.41×10^4	3.31×10^4	2.18×10^4	3.55×10^4
$\delta^+(\text{K-HMHC})\text{-AM}^{\delta-}$				
AM ⁺ = Be	1.06×10^4	1.36×10^4	1.65×10^4	2.02×10^4
AM ⁺ = Mg	1.57×10^4	1.26×10^4	2.46×10^4	2.82×10^4
AM ⁺ = Ca	2.58×10^4	3.54×10^4	2.71×10^4	3.90×10^4

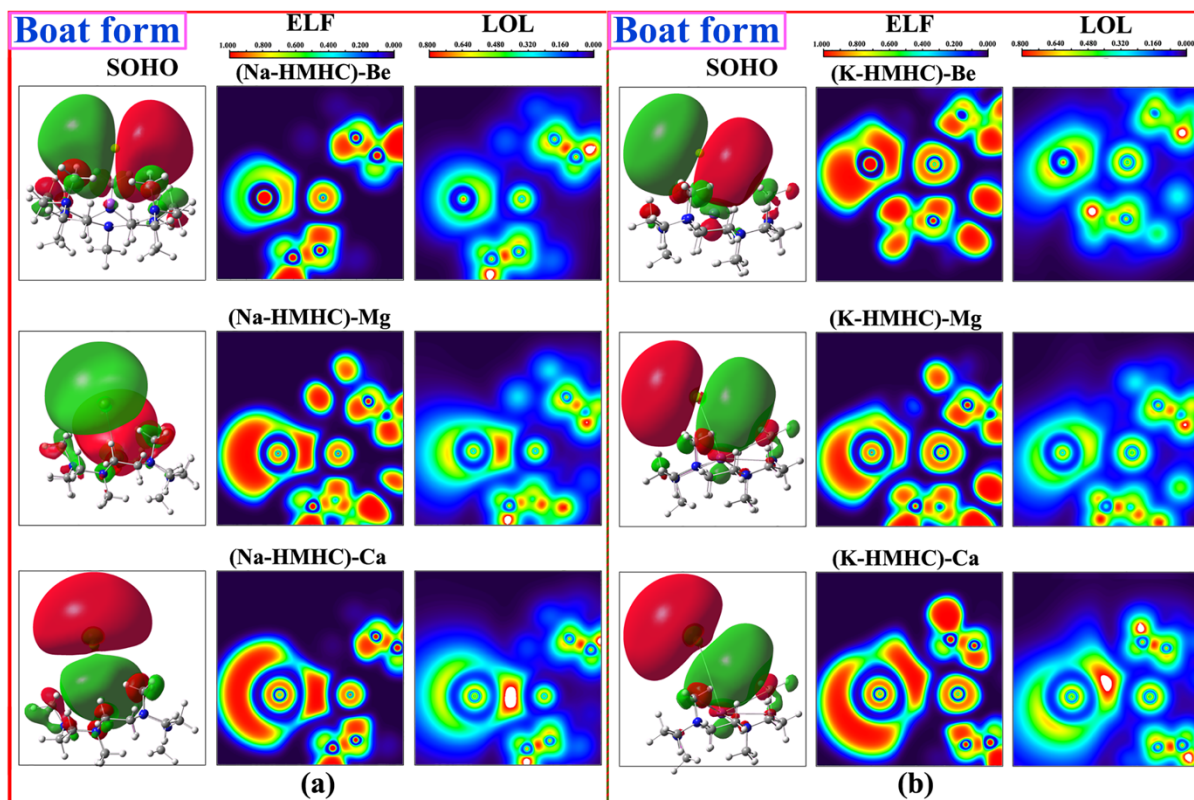


Fig. S1. SOMO and ELF as well as LOL maps for chair forms: (a) $\delta^+(\text{Na-HMHC})\text{-AM}'\delta^-$ and (b) $\delta^+(\text{K-HMHC})\text{-AM}'\delta^-$, ($\text{AM}' = \text{Be, Mg \& Ca}$).

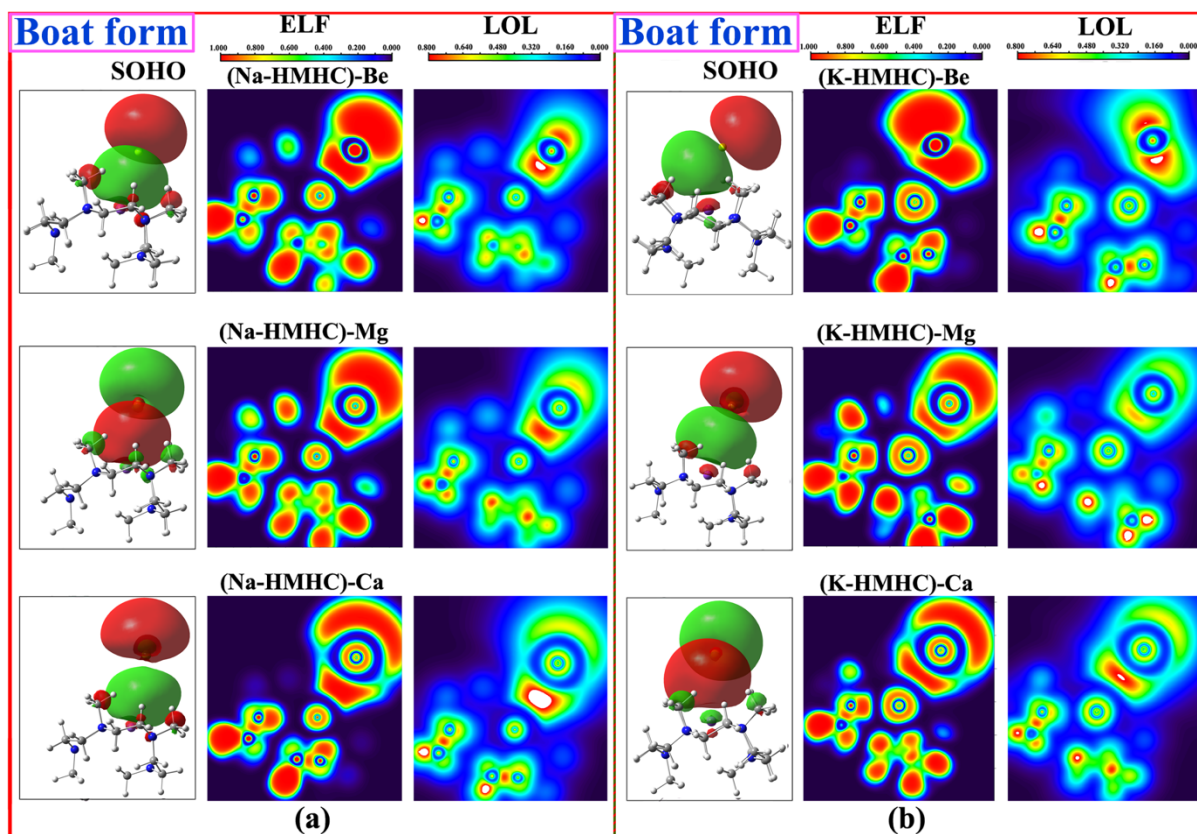


Fig. S2. SOMO and ELF as well as LOL maps for boat forms: (a) $\delta^+(\text{Na-HMHC})\text{-AM}'\delta^-$ and (b) $\delta^+(\text{K-HMHC})\text{-AM}'\delta^-$, (AM' = Be, Mg & Ca).

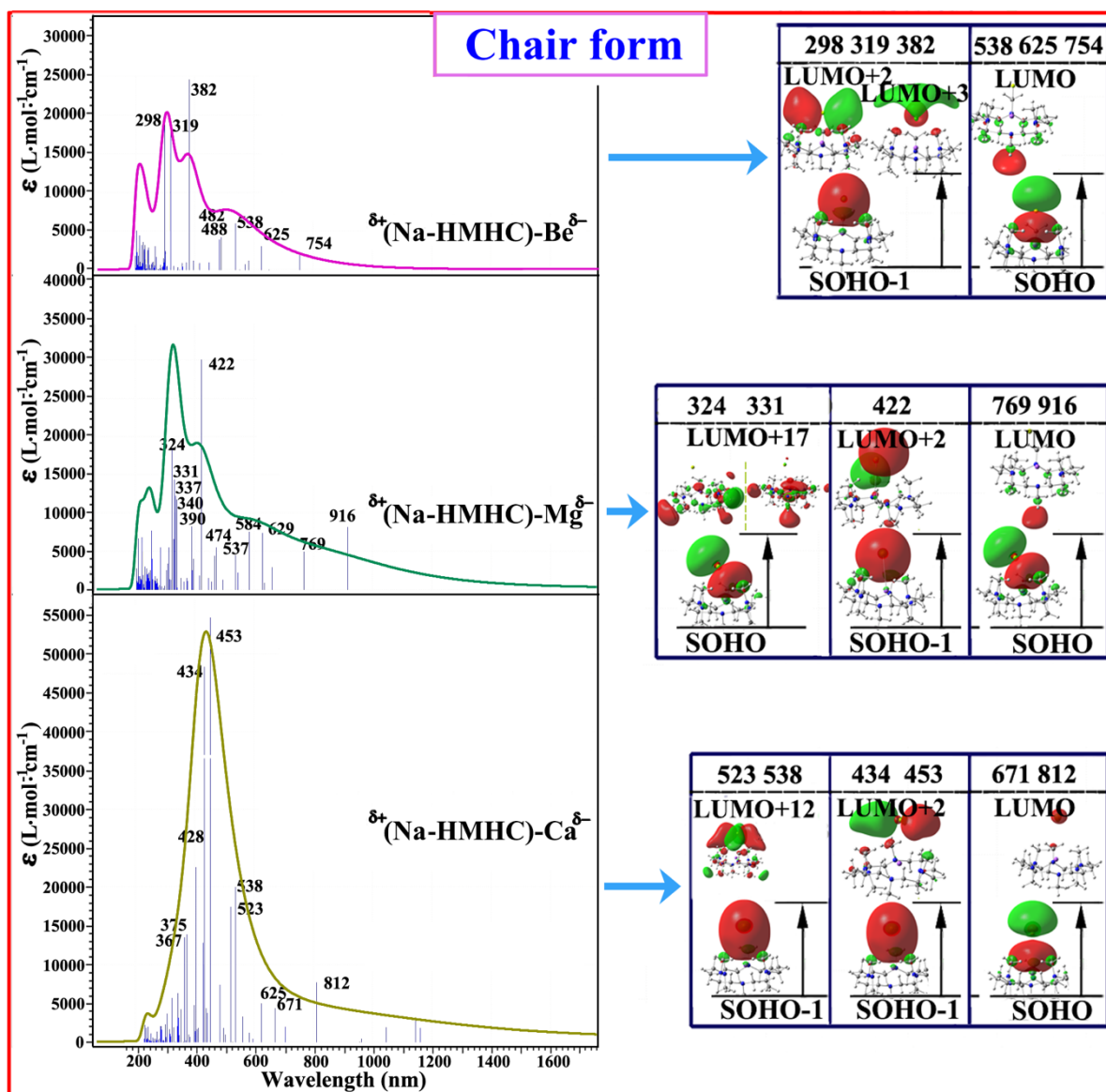


Fig. S3. Electronic absorption spectra of chair forms of $\delta^+(\text{Na-HMHC})\text{-AM}'^{\delta^-}$, (AM' = Be, Mg & Ca).

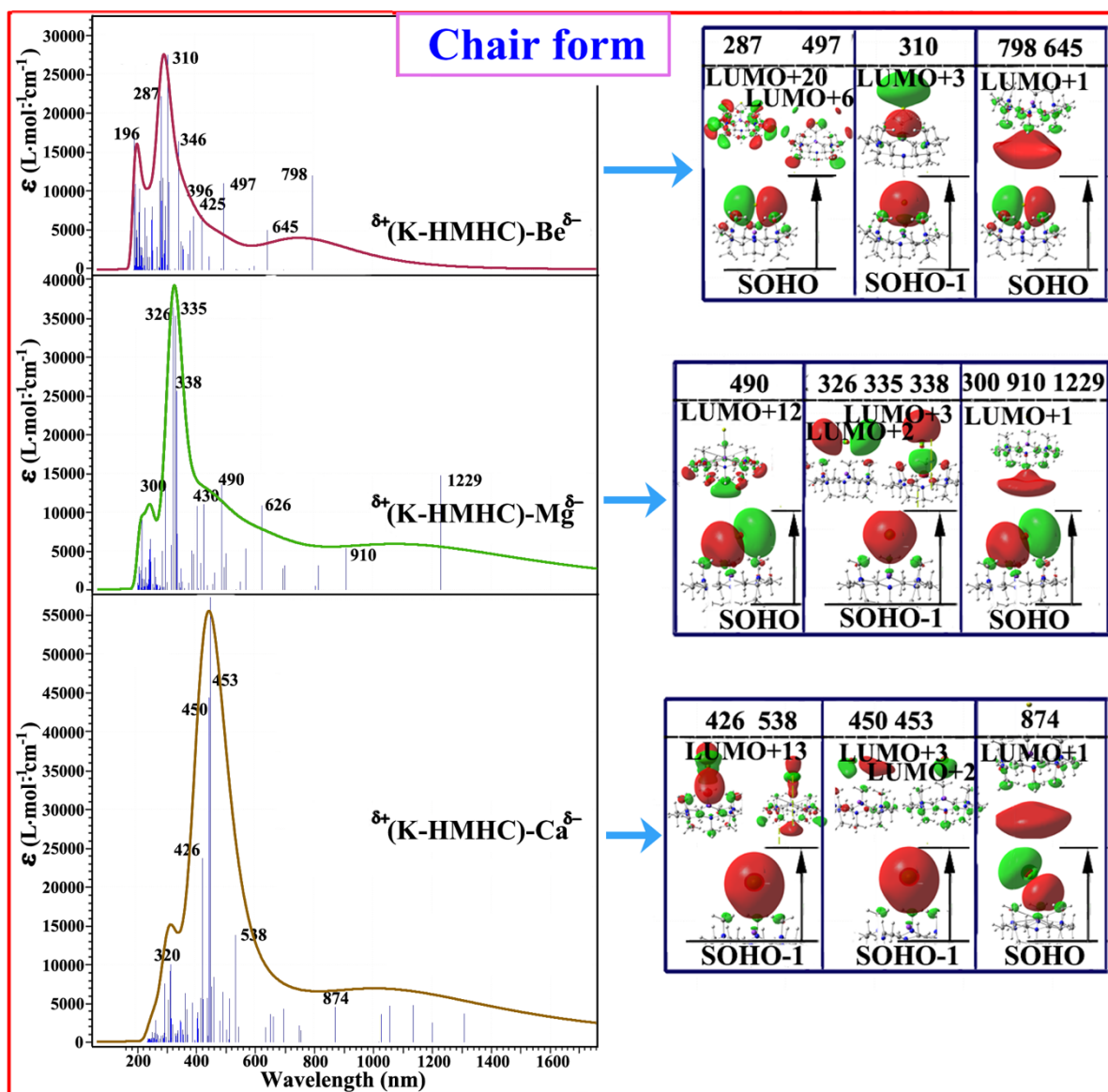


Fig. S4. Electronic absorption spectra of chair forms of $\delta^+(\text{K-HMHC})\text{-AM}'\delta^-$, ($\text{AM}' = \text{Be}, \text{Mg} \& \text{Ca}$).

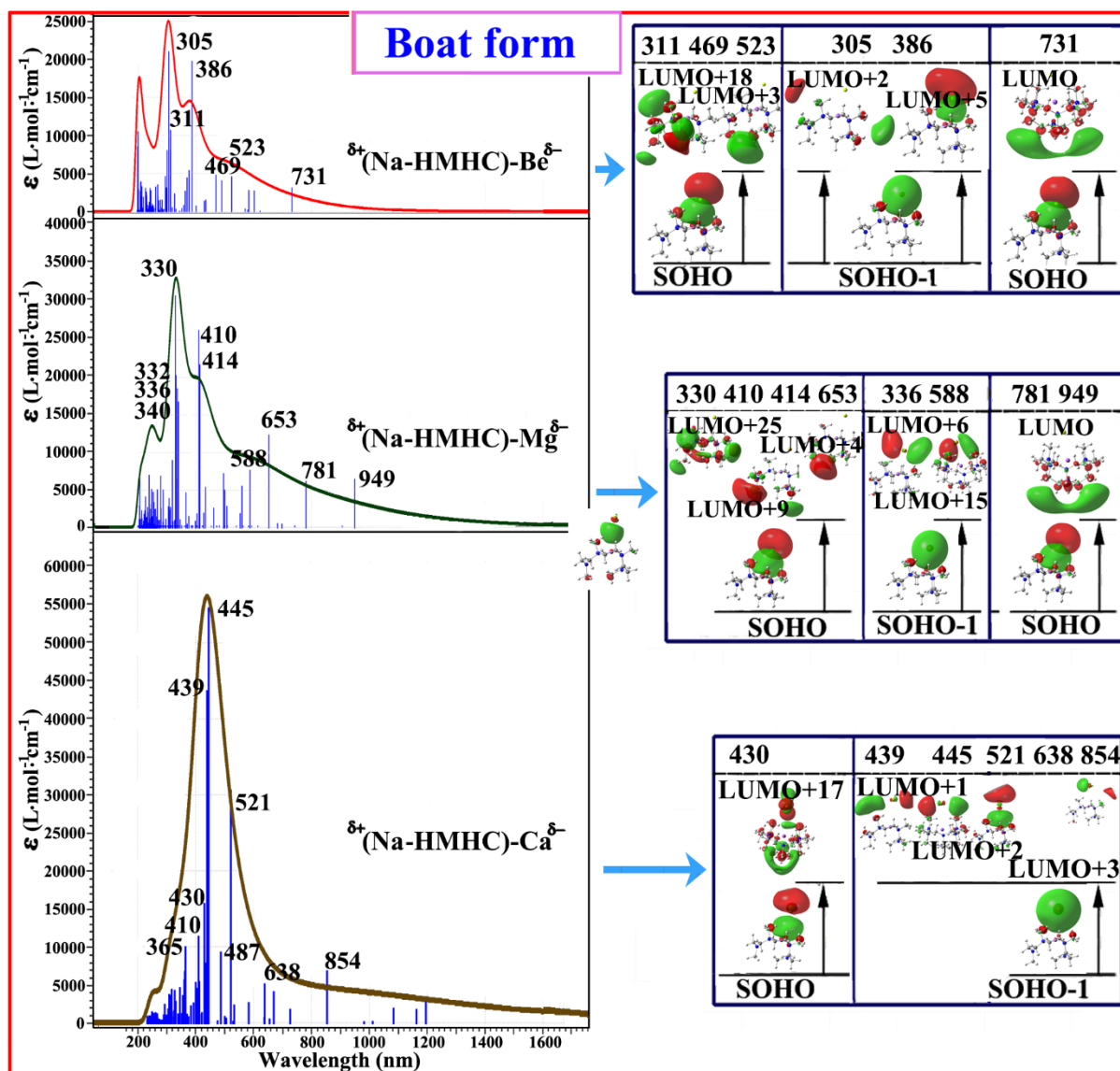


Fig. S5. Electronic absorption spectra of boat forms of δ^+ (Na-HMHC)-AM δ^- , (AM δ^- = Be, Mg & Ca).

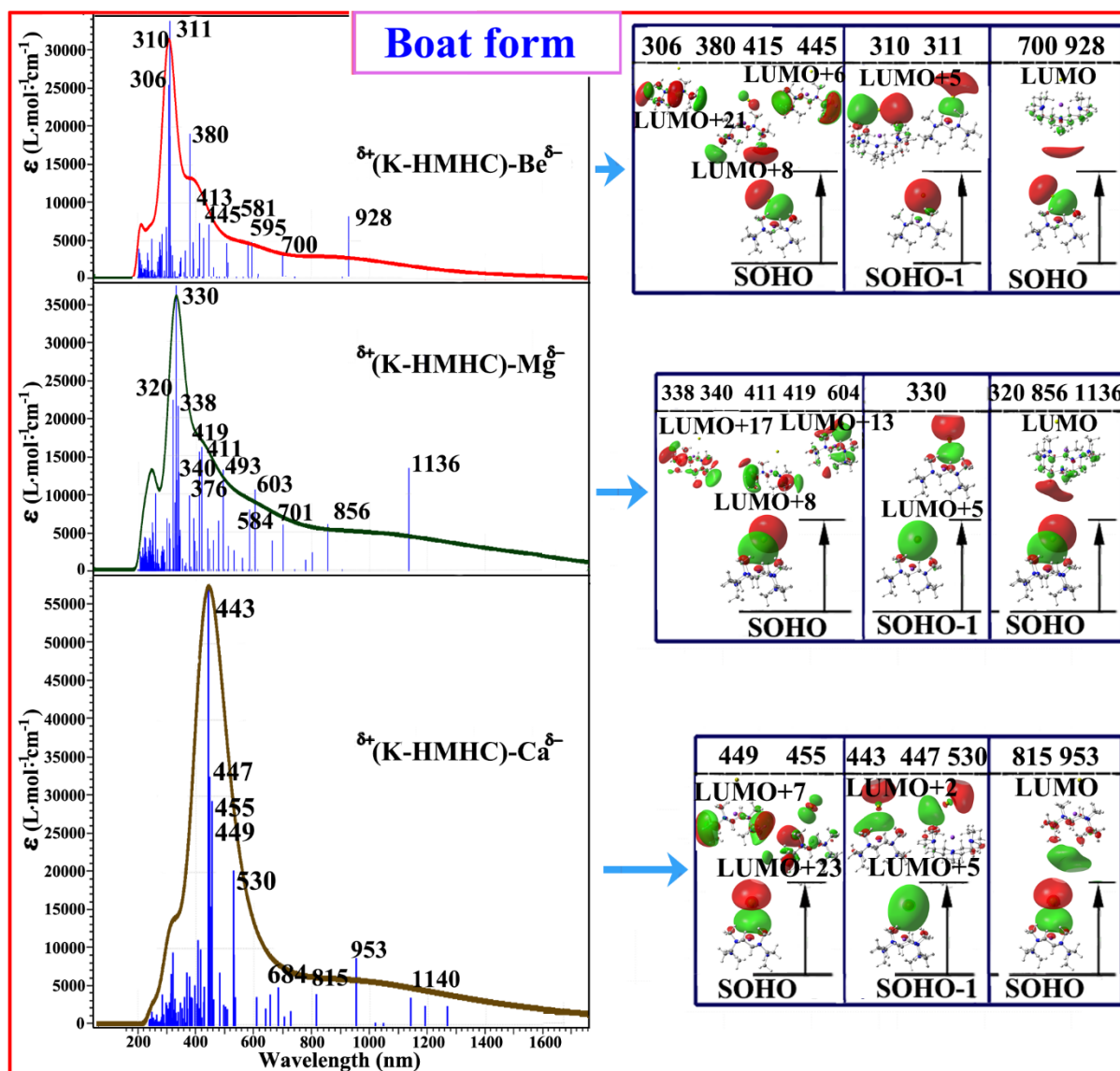


Fig. S6. Electronic absorption spectra of boat forms of $\delta^+(\text{K-HMHC})\text{-AM}'^{\delta^-}$, ($\text{AM}' = \text{Be}, \text{Mg} \& \text{Ca}$).