Supplementary Information

Transition metal chemistry in synthetically viable alkaline earth complexes $M(Cp)_3^-$ (M = Ca, Sr, Ba)

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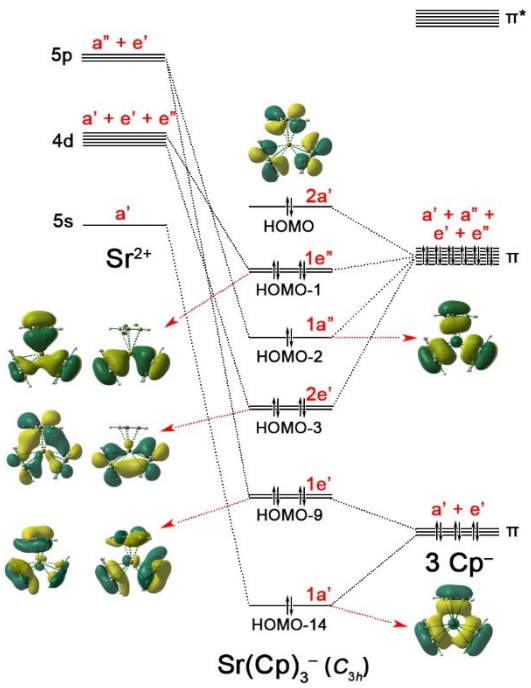

Fig. S1. MO correlation diagram of Sr^{2+} with three Cp^- ligands.

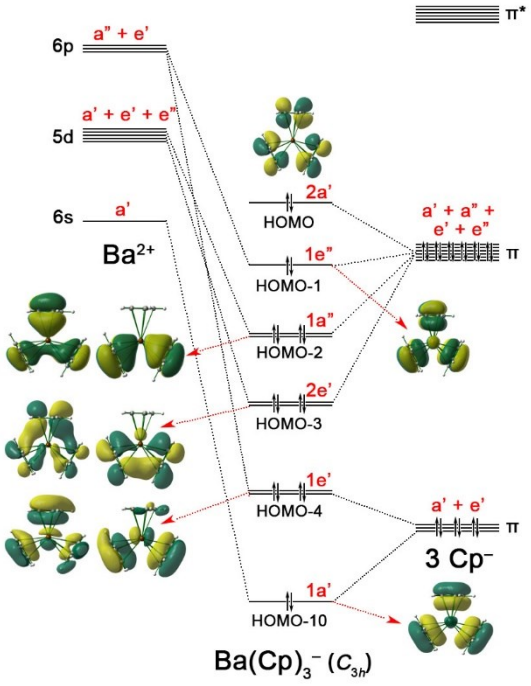

Fig. S2 MO correlation diagram of Ba^{2+} with three Cp^- ligands.

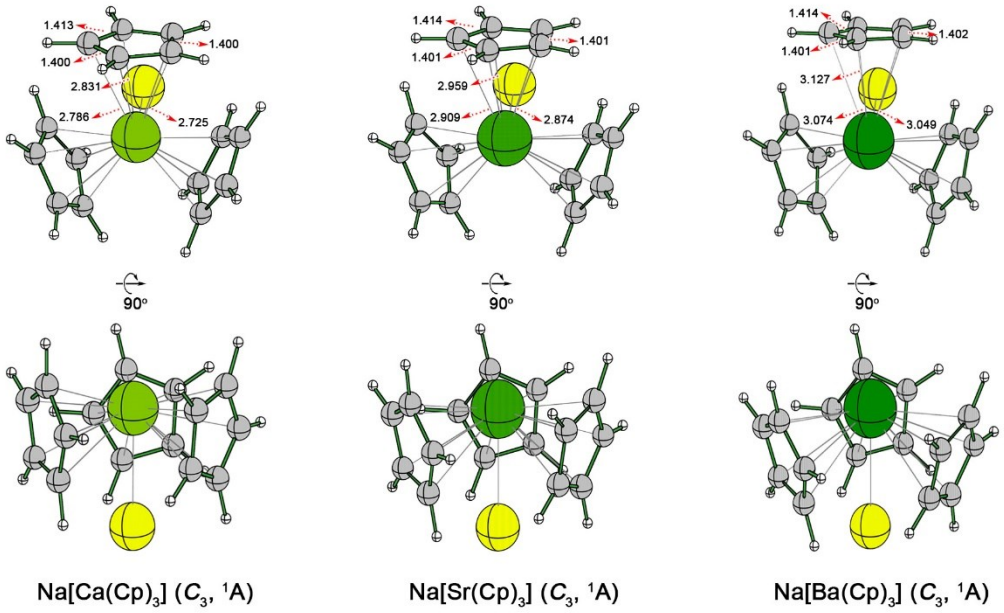

Fig. S3. Optimized structures of $Na[M(Cp)_3]$ (M = Ca, Sr, Ba)

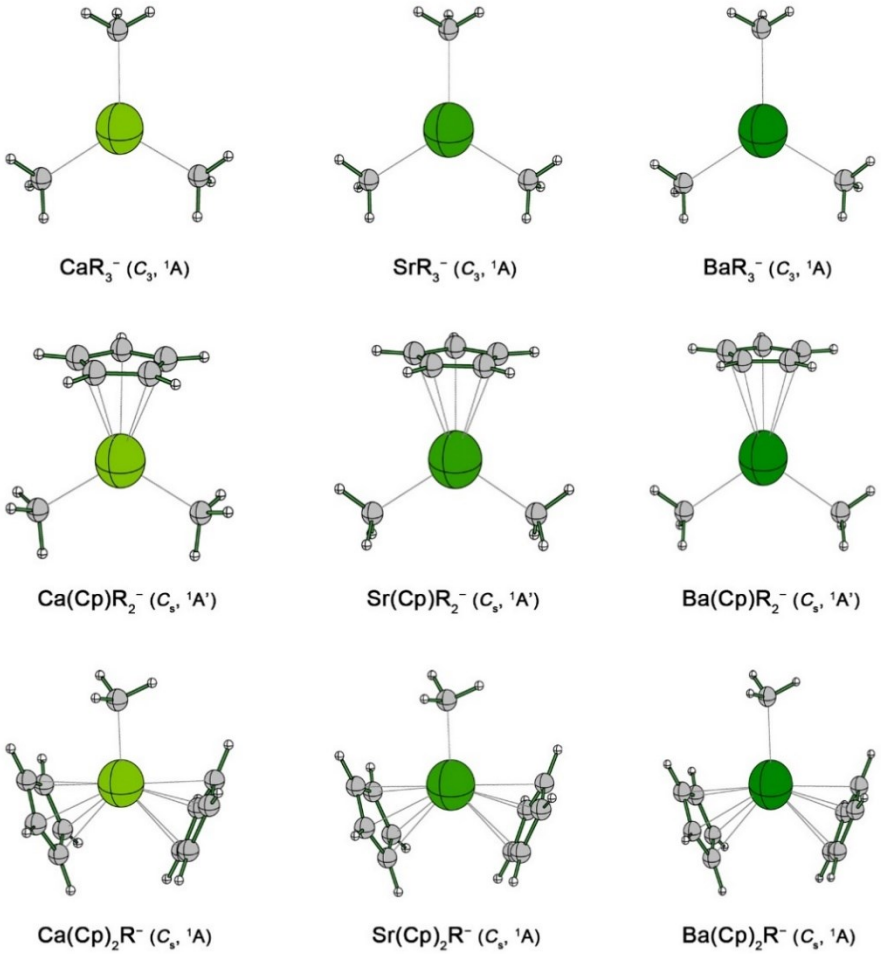

Fig. S4. Optimized structures of $M(Me)_3^-$, $M(Cp)(Me)_2^-$ and $M(Cp)_2(Me)^-$ (M = Ca, Sr, Ba)

Table S1. The lowest vibrational frequencies (ν_{min}) in cm^{-1}, the HOMO energy levels (E_{HOMO}), the HOMO-LUMO gaps (Gap), the VDEs and VEAs in eV, and the binding energies (BEs, in kcal/mol) at the M06-2X-D3/def2-TZVPP level. The BEs were calculated in three manners: regarding free positive metal centre and negative ligands (BE_{Tot}), regarding neutral metal, two neutral ligands and a negative Me anion (BE_{neu}), and regarding binding a Me^- by a $M(Me)_2$, M(Cp)Me, or $M(Cp)_2$ (BE_{Me}).

	ν_{min}	E_{HOMO}	Gap	VDE	VEA	BE_{Tot}	BE_{neu}	BE_{Me}
C_3 $Ca(Me)_3^-$	33	–2.32	5.79	3.37	4.43	–564.8	–145.4	–71.2
C_3 $Sr(Me)_3^-$	45	–2.19	5.26	3.22	3.95	–527.0	–134.9	–66.9
C_3 $Ba(Me)_3^-$	24	–2.05	4.58	3.03	3.27	–492.1	–135.8	–56.9
C_s $Ca(Cp)(Me)_2^-$	9	–2.28	5.68	3.27	4.46	–554.2	–64.4	–134.8
C_s $Sr(Cp)(Me)_2^-$	2	–2.19	5.27	3.17	3.98	–520.3	–64.5	–128.2
C_s $Ba(Cp)(Me)_2^-$	10	–2.07	4.57	3.00	3.24	–486.2	–60.4	–129.9
C_s $Ca(Cp)_2Me^-$	10	–2.43	5.73	3.33	4.26	–542.0	–149.7	–60.1
C_s $Sr(Cp)_2Me^-$	7	–2.37	5.41	3.27	3.96	–510.2	–145.3	–60.6
C_s $Ba(Cp)_2Me^-$	8	–2.23	4.68	3.09	3.19	–479.1	–150.0	–58.3

Formula S1: Reduction potential calculation formula

$$K = \exp\left(\frac{-\Delta G}{RT}\right) \qquad (1)$$

$$E = E^{\theta} - \frac{0.059 \log K}{2} \qquad (2)$$

Cartesian Coordinates for the structures shown in Fig. 1 .

M06-2X-D3/def2-TZVPP-optimized structures (in Cartesian coordinates) for structures shown in Fig. 1

$Ca(Cp)_3^-$ (C_{3h},$^1A'$) $E_{CCSD(T)//M06\text{-}2X}$ = -1256.768262 a.u

C	-2.65722004	0.84824764	0.00000000
H	-3.39330093	0.05957625	0.00000000
C	-2.07270604	1.43241595	1.13930900
H	-2.31105745	1.19648429	2.16648900
C	-1.13792535	2.39788602	0.70302300
H	-0.51760481	3.01272008	1.33761300
C	-2.07270604	1.43241595	-1.13930900
H	-2.31105745	1.19648429	-2.16648900
C	-1.13792535	2.39788602	-0.70302300
H	-0.51760481	3.01272008	-1.33761300
C	2.64559288	-0.21347075	-0.70302300
H	2.86789453	-1.05810112	-1.33761300
C	2.64559288	-0.21347075	0.70302300
H	2.86789453	-1.05810112	1.33761300
C	2.27686162	1.07880811	1.13930900
H	2.19171452	1.40319232	2.16648900
C	2.27686162	1.07880811	-1.13930900
H	2.19171452	1.40319232	-2.16648900
C	2.06321403	1.87709624	0.00000000
H	1.74824501	2.90889669	0.00000000
C	-1.50766753	-2.18441527	-0.70302300
H	-2.35028972	-1.95461896	-1.33761300
C	-1.50766753	-2.18441527	0.70302300
H	-2.35028972	-1.95461896	1.33761300
C	-0.20415558	-2.51122406	1.13930900
H	0.11934293	-2.59967661	2.16648900
C	-0.20415558	-2.51122406	-1.13930900
H	0.11934293	-2.59967661	-2.16648900
C	0.59400602	-2.72534388	0.00000000
H	1.64505592	-2.96847294	0.00000000
Ca	-0.00000000	0.00000000	0.00000000

$Sr(Cp)_3^-$ (C_{3h},$^1A'$) $E_{CCSD(T)//M06\text{-}2X}$ = -610.3691527 a.u

C	-1.64403110	-2.39738608	0.00000000
H	-1.07967900	-3.31760479	0.00000000
C	-2.06187150	-1.68274527	1.13952600
H	-1.90306618	-1.97856807	2.16679200
C	-2.74991004	-0.52853861	0.70334100
H	-3.19125363	0.22679822	1.33685200
C	-2.06187150	-1.68274527	-1.13952600
H	-1.90306618	-1.97856807	-2.16679200
C	-2.74991004	-0.52853861	-0.70334100
H	-3.19125363	0.22679822	-1.33685200
C	0.91722716	2.64576126	-0.70334100
H	1.79203984	2.65030761	-1.33685200
C	0.91722716	2.64576126	0.70334100
H	1.79203984	2.65030761	1.33685200
C	-0.42636441	2.62700573	1.13952600
H	-0.76195712	2.63738770	2.16679200
C	-0.42636441	2.62700573	-1.13952600
H	-0.76195712	2.63738770	-2.16679200
C	-1.25418170	2.62246574	0.00000000
H	-2.33329053	2.59383184	0.00000000
C	1.83268289	-2.11722265	-0.70334100
H	1.39921380	-2.87710583	-1.33685200
C	1.83268289	-2.11722265	0.70334100
H	1.39921380	-2.87710583	1.33685200
C	2.48823590	-0.94426046	1.13952600
H	2.66502331	-0.65881962	2.16679200
C	2.48823590	-0.94426046	-1.13952600
H	2.66502331	-0.65881962	-2.16679200
C	2.89821280	-0.22507966	0.00000000
H	3.41296953	0.72377296	0.00000000
Sr	0.00000000	-0.00000000	-0.00000000

$Ba(Cp)_3^-$ (C_{3h},$^1A'$) $E_{CCSD(T)//M06\text{-}2X}$ = -605.1557864 a.u

C	-2.33768020	1.99218541		0.00000000
H	-3.30305064	1.50780163		0.00000000
C	-1.59423551	2.35788323		1.13932600
H	-1.90368912	2.22687937		2.16673200
C	-0.39177631	2.95579184		0.70353600
H	0.39034597	3.34944558		1.33662600
C	-1.59423551	2.35788323		-1.13932600
H	-1.90368912	2.22687937		-2.16673200
C	-0.39177631	2.95579184		-0.70353600
H	0.39034597	3.34944558		-1.33662600
C	2.75567898	-1.13860768		-0.70353600
H	2.70553197	-2.01277232		-1.33662600
C	2.75567898	-1.13860768		0.70353600
H	2.70553197	-2.01277232		1.33662600
C	2.83910453	0.20170683		1.13932600
H	2.88037866	0.53520345		2.16673200
C	2.83910453	0.20170683		-1.13932600
H	2.88037866	0.53520345		-2.16673200
C	2.89412327	1.02839774		0.00000000
H	2.95731983	2.10662495		0.00000000
C	-2.36390266	-1.81718416		-0.70353600
H	-3.09587794	-1.33667326		-1.33662600
C	-2.36390266	-1.81718416		0.70353600
H	-3.09587794	-1.33667326		1.33662600
C	-1.24486902	-2.55959006		1.13932600
H	-0.97668954	-2.76208282		2.16673200
C	-1.24486902	-2.55959006		-1.13932600
H	-0.97668954	-2.76208282		-2.16673200
C	-0.55644307	-3.02058315		0.00000000
H	0.34573081	-3.61442658		0.00000000
Ba	0.00000000	0.00000000	-	0.00000000

$Ca(Cp)_2$ (C_2,^{1}A) $E_{CCSD(T)//M06\text{-}2X}$ = -1063.505155 a.u

C	0.58755847	-1.11806304	2.12920172
H	1.11500836	-2.05088704	2.00090007
C	-0.81465086	-0.95559104	2.15662453
H	-1.54571422	-1.74301104	2.05431470
C	-1.09177396	0.40909296	2.39129577
H	-2.07200604	0.84598096	2.50931651
C	1.17814299	0.14597896	2.34673318
H	2.23612372	0.34689696	2.42279765
C	0.14008994	1.09088196	2.50805648
H	0.26626360	2.13842196	2.73744694
C	1.09177396	0.40909296	-2.39129577
H	2.07200604	0.84598096	-2.50931651
C	-0.14008994	1.09088196	-2.50805648
H	-0.26626360	2.13842196	-2.73744694
C	-1.17814299	0.14597896	-2.34673318
H	-2.23612372	0.34689696	-2.42279765
C	0.81465086	-0.95559104	-2.15662453
H	1.54571422	-1.74301104	-2.05431470
C	-0.58755847	-1.11806304	-2.12920172
H	-1.11500836	-2.05088704	-2.00090007
Ca	0.00000000	0.30287996	0.00000000

$Sr(Cp)_2$ (C_2,^{1}A) $E_{CCSD(T)//M06\text{-}2X}$ = -417.094155 a.u

C	0.43541602	2.13918783	-1.30495226
H	0.82601855	1.90583606	-2.28386226
C	-0.92969186	2.23468240	-0.95905026
H	-1.76402395	2.09105206	-1.62904826
C	-1.01046792	2.61233986	0.39863274
H	-1.91816165	2.81880022	0.94634674
C	1.19865473	2.45775365	-0.16140926
H	2.27576119	2.52101821	-0.11599626
C	0.30528874	2.74943549	0.89247474
H	0.57959699	3.08276386	1.88256974
C	1.01046792	-2.61233986	0.39863274
H	1.91816165	-2.81880022	0.94634674
C	-0.30528874	-2.74943549	0.89247474
H	-0.57959699	-3.08276386	1.88256974
C	-1.19865473	-2.45775365	-0.16140926
H	-2.27576119	-2.52101821	-0.11599626
C	0.92969186	-2.23468240	-0.95905026
H	1.76402395	-2.09105206	-1.62904826
C	-0.43541602	-2.13918783	-1.30495226
H	-0.82601855	-1.90583606	-2.28386226
Sr	-0.00000000	0.00000000	0.42135874

$Ba(Cp)_2$ (C_2,^{1}A) $E_{CCSD(T)//M06\text{-}2X}$ = -411.8770867 a.u

C	-0.45810186	-1.97850586	-1.49249702
H	-0.86897098	-1.56918752	-2.40315402
C	0.91301241	-2.12329590	-1.19513602
H	1.73284812	-1.85019423	-1.84288002
C	1.02215902	-2.74505692	0.06673298
H	1.94199284	-3.04078907	0.55013598
C	-1.19576255	-2.50889926	-0.41382102
H	-2.27160798	-2.59164785	-0.36246702
C	-0.28070108	-2.98226987	0.55078498
H	-0.53392907	-3.49522631	1.46716198
C	-1.02215902	2.74505692	0.06673298
H	-1.94199284	3.04078907	0.55013598
C	0.28070108	2.98226987	0.55078498
H	0.53392907	3.49522631	1.46716198
C	1.19576255	2.50889926	-0.41382102
H	2.27160798	2.59164785	-0.36246702
C	-0.91301241	2.12329590	-1.19513602
H	-1.73284812	1.85019423	-1.84288002
C	0.45810186	1.97850586	-1.49249702
H	0.86897098	1.56918752	-2.40315402
Ba	-0.00000000	0.00000000	0.62481498

Cartesian Coordinates for the structures shown in Table. 1

M06-2X-D3/def2-TZVPP-optimized structures (in Cartesian coordinates) for structures shown in Table.1

$Ca(Bz)_3$ (D_3,^{1}A) $E_{M06\text{-}2X\text{-}D3/def2\text{-}TZVPP}$ = -1374.302095 a.u

C	-1.34102700	2.45207701	0.39267899
C	-1.01194400	2.45370001	-0.95401900
C	0.31695601	2.37844901	-1.37775700
C	1.34102700	2.45207701	-0.39267899
C	1.01194400	2.45370001	0.95401900
C	-0.31695601	2.37844901	1.37775700
H	-2.37543100	2.51796001	0.69409699
H	-1.80057599	2.47758101	-1.69535401
H	0.55831901	2.40175601	-2.42930100
H	2.37543100	2.51796001	-0.69409699
H	1.80057599	2.47758101	1.69535401
H	-0.55831901	2.40175601	2.42930100
C	1.45304748	-2.38740196	-0.39267899
C	1.61899455	-2.10321921	0.95401900
C	2.21827527	-0.91473255	1.37775700
C	2.79407449	-0.06467506	0.39267899
C	2.63093854	-0.35048080	-0.95401900
C	1.90131926	-1.46371646	-1.37775700
H	0.99290184	-3.31616360	-0.69409699
H	1.24536010	-2.79813506	1.69535401
H	2.35914123	-0.71735956	2.42930100
H	3.36833284	0.79820359	0.69409699
H	3.04593609	0.32055404	-1.69535401
H	1.80082222	-1.68439645	-2.42930100
C	-2.63093854	-0.35048080	0.95401900
C	-1.90131926	-1.46371646	1.37775700
C	-1.45304748	-2.38740196	0.39267899
C	-1.61899455	-2.10321921	-0.95401900
C	-2.21827527	-0.91473255	-1.37775700
C	-2.79407449	-0.06467506	-0.39267899
H	-3.04593609	0.32055404	1.69535401
H	-1.80082222	-1.68439645	2.42930100
H	-0.99290184	-3.31616360	0.69409699
H	-1.24536010	-2.79813506	-1.69535401
H	-2.35914123	-0.71735956	-2.42930100
H	-3.36833284	0.79820359	-0.69409699
Ca	-0.00000000	-0.00000000	0.00000000

$Sr(Bz)_3$ (D_3,^{1}A) $E_{M06\text{-}2X\text{-}D3/def2\text{-}TZVPP}$ = -727.368998 a.u

C	-0.32407699	2.52612306	1.37638500
C	1.00766100	2.57596106	0.96056300
C	1.34539300	2.56228206	-0.38651701
C	0.32407699	2.52612306	-1.37638500
C	-1.00766100	2.57596106	-0.96056300
C	-1.34539300	2.56228206	0.38651701
H	-0.57109099	2.56256006	2.42639800
H	1.79316701	2.59800906	1.70559199
H	2.38313100	2.60993806	-0.68203301
H	0.57109099	2.56256006	-2.42639800
H	-1.79316701	2.59800906	-1.70559199
H	-2.38313100	2.60993806	0.68203301
C	1.72701722	-2.16064056	0.96056300
C	2.34972524	-0.98240262	1.37638500
C	2.89169786	-0.11599652	0.38651701
C	2.73467822	-0.41532050	-0.96056300
C	2.02564825	-1.54372044	-1.37638500
C	1.54630486	-2.44628555	-0.38651701
H	1.35335834	-2.85193271	1.70559199
H	2.50478761	-0.78670073	2.42639800
H	3.45183816	0.75888295	0.68203301
H	3.14652535	0.25392365	-1.70559199
H	1.93369662	-1.77585934	-2.42639800
H	1.06870716	-3.36882101	-0.68203301
C	-2.73467822	-0.41532050	0.96056300
C	-2.02564825	-1.54372044	1.37638500
C	-1.54630486	-2.44628555	0.38651701
C	-1.72701722	-2.16064056	-0.96056300
C	-2.34972524	-0.98240262	-1.37638500
C	-2.89169786	-0.11599652	-0.38651701
H	-3.14652535	0.25392365	1.70559199
H	-1.93369662	-1.77585934	2.42639800
H	-1.06870716	-3.36882101	0.68203301
H	-1.35335834	-2.85193271	-1.70559199
H	-2.50478761	-0.78670073	-2.42639800
H	-3.45183816	0.75888295	-0.68203301
Sr	-0.00000000	-0.00000000	0.00000000

$Ba(Bz)_3$ (D_3,^{1}A) $E_{M06\text{-}2X\text{-}D3/def2\text{-}TZVPP}$ = -722.143010 a.u

C	-0.43465993	2.74160198	1.34068202
C	0.92268006	2.76376898	1.04533195
C	1.37424098	2.73165698	-0.27585208
C	0.43465993	2.74160198	-1.34068202
C	-0.92268006	2.76376898	-1.04533195
C	-1.37424098	2.73165698	0.27585208
H	-0.76848887	2.78231598	2.36730804
H	1.64227610	2.78718398	1.85435691
H	2.43268497	2.77303298	-0.48703813
H	0.76848887	2.78231598	-2.36730804
H	-1.64227610	2.78718398	-1.85435691
H	-2.43268497	2.77303298	0.48703813
C	1.93215412	-2.18094886	1.04533195
C	2.59162692	-0.99437445	1.34068202
C	3.05280483	-0.17570089	0.27585208
C	2.85483417	-0.58282012	-1.04533195
C	2.15696700	-1.74722753	-1.34068202
C	1.67856385	-2.55595609	-0.27585208
H	1.59263408	-2.81584481	1.85435691
H	2.79380075	-0.72562711	2.36730804
H	3.61785949	0.72025050	0.48703813
H	3.23491018	0.02866084	-1.85435691
H	2.02531188	-2.05668887	-2.36730804
H	1.18517452	-3.49328348	-0.48703813
C	-2.85483417	-0.58282012	1.04533195
C	-2.15696700	-1.74722753	1.34068202
C	-1.67856385	-2.55595609	0.27585208
C	-1.93215412	-2.18094886	-1.04533195
C	-2.59162692	-0.99437445	-1.34068202
C	-3.05280483	-0.17570089	-0.27585208
H	-3.23491018	0.02866084	1.85435691
H	-2.02531188	-2.05668887	2.36730804
H	-1.18517452	-3.49328348	0.48703813
H	-1.59263408	-2.81584481	-1.85435691
H	-2.79380075	-0.72562711	-2.36730804
H	-3.61785949	0.72025050	-0.48703813
Ba	0.00000000	0.00000000	-0.00000000

Na[Ca(Cp)$_3$] (C_3,^{1}A) $E_{CCSD(T)//M06\text{-}2X}$ = -1418.769832 a.u

C	2.02346452	1.86825099	0.17664990
H	1.73707209	2.90654370	0.21368391
C	2.39505228	1.07483051	1.26884089
H	2.46848354	1.40634430	2.29410989
C	2.70896853	-0.22106596	0.78894088
H	3.04139892	-1.05669092	1.38476887
C	2.09046423	1.06868075	- 0.98656210
H	2.02708510	1.45184263	-2.00042410
C	2.53497591	-0.22153368	-0.60071611
H	2.73650183	-1.05483842	-1.25798612
C	-1.45934175	-2.08458669	-0.60071611
H	-2.28176778	-1.84246089	-1.25798612
C	-1.54593300	-2.23550259	0.78894088
H	-2.43582064	-2.10558327	1.38476887
C	-0.26669562	-2.61159137	1.26884089
H	-0.01631188	-2.84094160	2.29410989
C	-0.11972744	-2.34473551	-0.98656210
H	0.24379005	-2.48142851	-2.00042410
C	0.60622056	-2.68649717	0.17664990
H	1.64860463	-2.95762041	0.21368391
C	-1.07563416	2.30612038	-0.60071611
H	-0.45473404	2.89729931	-1.25798612
C	-1.16303553	2.45656854	0.78894088
H	-0.60557828	3.16227419	1.38476887
C	-2.12835666	1.53676087	1.26884089
H	-2.45217166	1.43459731	2.29410989
C	-1.97073680	1.27605476	-0.98656210
H	-2.27087515	1.02958588	-2.00042410
C	-2.62968508	0.81824618	0.17664990
H	-3.38567673	0.05107671	0.21368391
Na	-0.00000000	0.00000000	-2.31320207
Ca	-0.00000000	-0.00000000	0.59469993

$Na[Sr(Cp)_3]$ (C_3,^{1}A)	$E_{CCSD(T)//M06-2X}$ = -772.3680229 a.u		
C	1.72606374	-2.26344119	0.07530209
H	2.78401710	-2.06218693	0.13165512
C	0.90162736	-2.66684777	1.13376606
H	1.22245892	-2.85045618	2.14889006
C	-0.41141387	-2.84366473	0.63258002
H	-1.27159496	-3.16816899	1.19788099
C	0.92945106	-2.18644005	-1.09030193
H	1.32517767	-2.07907462	-2.09572392
C	-0.39171594	-2.56234718	-0.74005898
H	-1.23393127	-2.65854411	-1.41041700
C	-2.02319978	1.62040955	-0.74005898
H	-1.68540110	2.39788789	-1.41041700
C	-2.25697896	1.77812723	0.63258002
H	-2.10791735	2.68531804	1.19788099
C	-2.76037160	0.55259169	1.13376606
H	-3.07979693	0.36654761	2.14889006
C	-2.35823816	0.28829180	-1.09030193
H	-2.46312027	-0.10810022	-2.09572392
C	-2.82322944	-0.36309445	0.07530209
H	-3.17791482	-1.37993606	0.13165512
C	2.41491572	0.94193763	-0.74005898
H	2.91933237	0.26065623	-1.41041700
C	2.66839284	1.06553750	0.63258002
H	3.37951231	0.48285095	1.19788099
C	1.85874424	2.11425609	1.13376606
H	1.85733801	2.48390857	2.14889006
C	1.42878710	1.89814826	-1.09030193
H	1.13794260	2.18717484	-2.09572392
C	1.09716570	2.62653564	0.07530209
H	0.39389773	3.44212300	0.13165512
Sr	0.00000000	-0.00000000	0.67335808
Na	0.00000000	-0.00000000	-2.33705792

$Na[Ba(Cp)_3]$ (C_3,^{1}A) $E_{CCSD(T)//M06\text{-}2X}$ = -767.1584035 a.u

C	1.95693800	2.21618300	-0.06666900
H	1.55048600	3.21304200	0.00613500
C	2.61734800	1.51112700	0.94861100
H	2.81829600	1.87933400	1.94445200
C	3.01855000	0.25661500	0.43170000
H	3.56857900	-0.50660200	0.96131500
C	1.95186100	1.40412000	-1.22363300
H	1.68057700	1.75749300	-2.21393100
C	2.62117300	0.19500500	-0.91150400
H	2.84136400	-0.61671800	-1.59075000
C	-1.14170700	-2.36750500	-0.91150400
H	-1.95477500	-2.15233500	-1.59075000
C	-1.28704000	-2.74244800	0.43170000
H	-2.22301900	-2.83717900	0.96131500
C	0.00000000	-3.02225300	0.94861100
H	0.21840300	-3.38038300	1.94445200
C	0.24007300	-2.39242100	-1.22363300
H	0.68174500	-2.33416900	-2.21393100
C	0.94080200	-2.80284900	-0.06666900
H	2.00733300	-2.94928100	0.00613500
C	-1.47946500	2.17250000	-0.91150400
H	-0.88658900	2.76905200	-1.59075000
C	-1.73151000	2.48583300	0.43170000
H	-1.34556000	3.34378100	0.96131500
C	-2.61734800	1.51112700	0.94861100
H	-3.03669900	1.50104900	1.94445200
C	-2.19193400	0.98830100	-1.22363300
H	-2.36232200	0.57667600	-2.21393100
C	-2.89774000	0.58666700	-0.06666900
H	-3.55781900	-0.26376100	0.00613500
Na	0.00000000	0.00000000	-2.35960100
Ba	0.00000000	0.00000000	0.77537300

Cartesian Coordinates for the structures shown in Fig.S4

M06-2X-D3/def2-TZVPP-optimized structures (in Cartesian coordinates) for structures shown in Fig.S4

$Ca(Me)_3$ (C_3,^{1}A) $E_{M06\text{-}2X\text{-}D3/def2\text{-}TZVPP}$ = -797.282607 a.u

C	0.00000000	2.52379000	0.00182100
H	-0.01928300	2.95511000	-1.01018800
H	0.88690400	2.95568000	0.48734100
H	-0.86923700	2.95430000	0.51957100
C	-2.18566700	-1.26189500	0.00182100
H	-3.00314600	-0.70975800	0.48734100
H	-2.12388000	-2.22993100	0.51957100
H	-2.54955900	-1.49425500	-1.01018800
C	2.18566700	-1.26189500	0.00182100
H	2.56884200	-1.46085500	-1.01018800
H	2.11624100	-2.24592200	0.48734100
H	2.99311700	-0.72436900	0.51957100
Ca	0.00000000	0.00000000	-0.00114800

$Sr(Me)_3$ (C_3,^{1}A) $E_{M06\text{-}2X\text{-}D3/def2\text{-}TZVPP}$ = -150.329358a.u

C	-0.02406591	2.68670533	0.00022778
H	-0.04490660	3.11540186	-1.01355122
H	0.85816359	3.12869123	0.48672978
H	-0.89806300	3.11195995	0.51572978
C	-2.31472211	-1.36419435	0.00022778
H	-3.13860788	-0.82115414	0.48672978
H	-2.24600487	-2.33372535	0.51572978
H	-2.67556385	-1.59659119	-1.01355122
C	2.33878802	-1.32251097	0.00022778
H	2.72047045	-1.51881067	-1.01355122
H	2.28044429	-2.30753708	0.48672978
H	3.14406787	-0.77823460	0.51572978
Sr	0.00000000	-0.00000000	0.00076777

$Ba(Me)_3$ (C_3,^{1}A) $E_{M06\text{-}2X\text{-}D3/def2\text{-}TZVPP}$ = -145.090523a.u

C	1.07853169	2.64440372	-0.04118793
H	1.27089585	3.04309937	0.96786007
H	0.41599525	3.37891078	-0.52392693
H	2.04132165	2.71302813	-0.57021393
C	1.75085496	-2.25623770	-0.04118793
H	2.71822494	-2.04971784	-0.52392693
H	1.32889046	-3.12435048	-0.57021393
H	1.99995344	-2.62217778	0.96786007
C	-2.82938664	-0.38816602	-0.04118793
H	-3.27084929	-0.42092160	0.96786007

H	-3.13422019	-1.32919293	-0.52392693
H	-3.37021211	0.41132234	-0.57021393
Ba	-0.00000000	0.00000000	0.02000404

$CaCp(Me)_2$ (C_s,^{1}A') $E_{M06\text{-}2X\text{-}D3/def2\text{-}TZVPP}$ = -950.962787a.u

C	-1.20071685	-1.61236105	0.00000000
C	-0.37195082	-1.61613589	1.14190400
H	-0.70289922	-1.59880169	2.16918200
C	0.96729342	-1.62104995	0.70612700
H	1.83912697	-1.62550025	1.34376500
C	-0.37195082	-1.61613589	-1.14190400
H	-0.70289922	-1.59880169	-2.16918200
C	0.96729342	-1.62104995	-0.70612700
H	1.83912697	-1.62550025	-1.34376500
H	-2.28120368	-1.62170828	0.00000000
C	-0.00065628	2.13860333	2.14945700
H	0.09789795	3.22489828	2.01652400
H	-0.92513206	1.98797093	2.72671200
H	0.81488814	1.83904396	2.82421900
C	-0.00065628	2.13860333	-2.14945700
H	-0.92513206	1.98797093	-2.72671200
H	0.09789795	3.22489828	-2.01652400
H	0.81488814	1.83904396	-2.82421900
Ca	0.00507527	0.84118211	0.00000000

$SrCp(Me)_2$ (C_s,^{1}A') $E_{M06\text{-}2X\text{-}D3/def2\text{-}TZVPP}$ = -304.012728a.u

C	-1.01697400	-2.02795400	0.00000000
C	-0.19183600	-1.95272400	1.14172600
H	-0.52187000	-1.98219900	2.16943200
C	1.14158400	-1.82836800	0.70594400
H	2.01146900	-1.76196500	1.34335700
C	-0.19183600	-1.95272400	-1.14172600
H	-0.52187000	-1.98219900	-2.16943200
C	1.14158400	-1.82836800	-0.70594400
H	2.01146900	-1.76196500	-1.34335700
H	-2.09083700	-2.15064700	0.00000000
C	-0.19183600	2.13300900	2.26622100
H	-1.04477200	2.82753600	2.28633100
H	-0.27953300	1.51926000	3.17389700
H	0.69953500	2.76115000	2.41409500
C	-0.19183600	2.13300900	-2.26622100
H	-0.27953300	1.51926000	-3.17389700
H	-1.04477200	2.82753600	-2.28633100

H	0.69953500	2.76115000	-2.41409500
Sr	-0.06926100	0.72020500	0.00000000

$BaCp(Me)_2$ (C_s,^{1}A') $E_{M06\text{-}2X\text{-}D3/def2\text{-}TZVPP}$ = -298.776119a.u

C	-1.64436600	-1.89171100	0.00000000
C	-0.83628200	-2.07372600	1.14150200
H	-1.16192700	-2.00908600	2.16946000
C	0.47096400	-2.36092900	0.70592000
H	1.31878500	-2.56914700	1.34308700
C	-0.83628200	-2.07372600	-1.14150200
H	-1.16192700	-2.00908600	-2.16946000
C	0.47096400	-2.36092900	-0.70592000
H	1.31878500	-2.56914700	-1.34308700
H	-2.70611800	-1.68775600	0.00000000
C	0.47096400	2.10836900	2.41995100
H	-0.28155800	2.90306100	2.54114900
H	0.40336900	1.49175500	3.32810400
H	1.44500100	2.61881500	2.47504000
C	0.47096400	2.10836900	-2.41995100
H	0.40336900	1.49175500	-3.32810400
H	-0.28155800	2.90306100	-2.54114900
H	1.44500100	2.61881500	-2.47504000
Ba	0.14030700	0.64433300	0.00000000

$Ca(Cp)_2Me$ (C_s,^1A) $E_{M06\text{-}2X\text{-}D3/def2\text{-}TZVPP}$ = -1104.641957 a.u

C	1.74867164	-1.61848243	0.00000000
H	1.29841551	-2.59973014	0.00000000
C	2.08347566	-0.86032193	1.14007900
H	1.95527937	-1.17070155	2.16708200
C	2.63066432	0.36618182	0.70338300
H	2.96887266	1.17428224	1.33415300
C	2.08347566	-0.86032193	-1.14007900
H	1.95527937	-1.17070155	-2.16708200
C	2.63066432	0.36618182	-0.70338300
H	2.96887266	1.17428224	-1.33415300
C	-2.37134737	-0.22491063	-1.13938300
H	-2.51659447	0.07753972	-2.16632200
C	-2.72485218	0.52477214	0.00000000
H	-3.15044498	1.51622865	0.00000000
C	-2.37134737	-0.22491063	1.13938300
H	-2.51659447	0.07753972	2.16632200
C	-1.80098812	-1.44131425	-0.70405800
H	-1.42535967	-2.23144304	-1.33736300
C	-1.80098812	-1.44131425	0.70405800
H	-1.42535967	-2.23144304	1.33736300
C	-0.07112979	2.98500444	0.00000000
H	-0.61258570	3.37656843	-0.87455000
H	-0.61258570	3.37656843	0.87455000
H	0.90982265	3.47974869	0.00000000
Ca	-0.00074047	0.48639381	0.00000000

$Sr(Cp)_2Me$ (C_s,^1A) $E_{M06\text{-}2X\text{-}D3/def2\text{-}TZVPP}$ = -457.696770 a.u

C	1.86115523	-1.74372994	0.00000000
H	1.39476434	-2.71780546	0.00000000
C	2.21459382	-0.99418032	1.13996800
H	2.08727072	-1.30554251	2.16703900
C	2.79054477	0.21897210	0.70373300
H	3.16388082	1.01169644	1.33494100
C	2.21459382	-0.99418032	-1.13996800
H	2.08727072	-1.30554251	-2.16703900
C	2.79054477	0.21897210	-0.70373300
H	3.16388082	1.01169644	-1.33494100
C	-2.51765016	-0.36585359	-1.13951900
H	-2.68003201	-0.07202732	-2.16669900
C	-2.88684274	0.37686120	0.00000000
H	-3.35293658	1.35044186	0.00000000
C	-2.51765016	-0.36585359	1.13951900
H	-2.68003201	-0.07202732	2.16669900

C	-1.92067732	-1.56867205	-0.70412700
H	-1.53511851	-2.35450029	-1.33729600
C	-1.92067732	-1.56867205	0.70412700
H	-1.53511851	-2.35450029	1.33729600
C	-0.07292741	3.13281444	0.00000000
H	-0.60789614	3.53063747	-0.87534300
H	-0.60789614	3.53063747	0.87534300
H	0.91421213	3.61560911	0.00000000
Sr	-0.00058667	0.47506208	0.00000000

$Ba(Cp)_2Me$ (C_s,^{1}A) $E_{M06\text{-}2X\text{-}D3/def2\text{-}TZVPP}$ = -452.463924 a.u

C	2.65066800	-0.80943100	0.00000000
H	2.65742100	-1.88976900	0.00000000
C	2.64797600	0.01919800	1.13959600
H	2.67304000	-0.31629500	2.16692600
C	2.64797600	1.36166000	0.70359100
H	2.65473400	2.23789800	1.33545500
C	2.64797600	0.01919800	-1.13959600
H	2.67304000	-0.31629500	-2.16692600
C	2.64797600	1.36166000	-0.70359100
H	2.65473400	2.23789800	-1.33545500
C	-2.25392700	-1.58014600	-1.13920700
H	-2.52843400	-1.38636900	-2.16660400
C	-2.89938400	-1.05922200	0.00000000
H	-3.73837800	-0.37936700	0.00000000
C	-2.25392700	-1.58014600	1.13920700
H	-2.52843400	-1.38636900	2.16660400
C	-1.21068700	-2.42451700	-0.70405900
H	-0.53909200	-2.98624700	-1.33742800
C	-1.21068700	-2.42451700	0.70405900
H	-0.53909200	-2.98624700	1.33742800
C	-1.42019300	2.94831900	0.00000000
H	-2.06676100	3.10817800	-0.87616100
H	-2.06676100	3.10817800	0.87616100
H	-0.69809800	3.77777900	0.00000000
Ba	-0.18875900	0.39615500	0.00000000