Supporting information for

Dimetallofullerene $M_2@C_{100}$ or Carbide Cluster Fullerene $M_2C_2@C_{98}$ (M= La, Y, Sc): Which Ones Are More Stable?

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Figure S2 NBO charge distributions of the most sable isomers of $M_2@C_{100}$ and $M_2C_2@C_{98}$ (M= La, Y, Sc). Green represents positive charge and red represents negative charge.

Figure S3 Simulated IR spectra of main M_2C_{100} isomers.

Table S1 Relative energies of C_{98}^{4-} optimized at AM1level.

Spiral ID	Symmetry	PA	△E (kcal/mol)
230925	C_{2v}	0	0
230924	C_2	0	0.27
230926	C_1	0	0.60
230933	C_1	0	0.69
230979	C_2	0	1.14
230927	C_1	0	3.23
230941	C_2	0	3.32
230839	C_1	0	3.44
230938	C_1	0	4.97
230931	C_1	0	5.43
230889	C_1	0	6.54
230932	C_2	0	6.63
230969	C_2	0	6.83
231005	C_1	0	7.19
230947	C_2	0	7.33
231004	C_2	0	7.79
230991	C_2	0	7.90
230930	C_1	0	7.93
230942	C_1	0	8.15
230830	C_2	0	8.73
230984	C_1	0	9.04
230992	C_1	0	10.21
230844	C_1	0	10.37
230919	C_1	0	10.53
230917	C_1	0	11.33
230902	C_1	0	11.36
230970	C_1	0	11.54
230982	C_1	0	11.60
230983	C_2	0	11.75
230895	C_1	0	11.77

230847	C_2	0	12.33
230883	C_1	0	12.39
230989	C_2	0	12.56
230944	C_1	0	12.63
231000	C_2	0	12.79
230963	C_s	0	12.80
230899	C_1	0	12.80
230882	C_1	0	13.35
230923	C_1	0	13.63
230898	C_1	0	13.65
230890	C_1	0	13.66
230903	C_1	0	13.69
230940	C_2	0	13.70
230905	C_2	0	13.75
230921	C_1	0	13.90
230833	C_1	0	14.31
230934	C_2	0	14.51
230937	C_1	0	14.93
230827	C_1	0	15.52
230901	C_1	0	15.73
230946	C_2	0	15.78
230832	C_2	0	15.79
230935	C_1	0	15.85
230879	C_1	0	15.87
230976	C_s	0	16.09
230928	C_1	0	16.36
230929	C_1	0	16.54
230985	C_1	0	16.55
230948	C_1	0	16.59
230966	C_1	0	16.81
230878	C_s	0	17.14
230600	C_1	1	18.04
219677	C_1	1	18.23
230943	C_s	0	18.30
231013	C_1	0	18.40

231002	C_1	0	18.44
230728	C_1	1	18.51
229418	C_1	1	18.55
231014	C_2	0	18.59
230837	C_1	0	19.24
219676	C_1	1	19.45
230877	C_s	0	19.46
230765	C_s	0	19.66
230872	C_1	0	19.68
220108	C_1	1	20.02
230953	C_1	0	20.15
172198	C_1	1	20.96
230962	C_1	0	20.97
230965	C_1	0	21.18
230981	C_1	0	21.29
170811	C_1	1	21.36
230880	C_1	0	21.48
229404	C_1	1	21.80
228592	C_1	1	21.79
230986	C_1	0	21.80
229416	C_1	1	21.81
230957	C_s	0	22.09
230975	C_1	0	22.36
231012	C_2	0	22.71
229408	C_1	1	22.73
229329	C_1	1	22.90
230599	C_1	1	22.92
231011	C_3	0	22.93
230859	C_1	0	22.99
230913	C_1	0	23.04
230977	C_1	0	23.15
229413	C_1	1	23.21
230912	C_1	0	23.36
219722	C_1	1	23.37
230470	C_1	1	23.47

Table S2 Relative energies and HOMO-LUMO Gaps of C_{98}^{4-} optimized at B3LYP/6-31G level.

Spiral ID	Symmetry	PA	△E(kcal/mol)	Gap(eV)
230979	C_2	0	0	1.41
230933	C_1	0	0.36	1.11
230926	C_1	0	0.70	1.19
230925	C_{2v}	0	0.74	1.24
230924	C_2	0	1.08	0.87
230927	C_1	0	3.33	1.43
230941	C_2	0	3.61	1.28
230839	C_1	0	4.42	1.41
230931	C_1	0	4.66	1.25
230979	C_2	0	4.70	1.31

Table S3 Coordinates of main M_2C_{100} isomers predicted at B3LYP/6-31G(d) ~ Lanl2dz level.

$La_2@D_5(285913)$-C_{100}

xyz file：

C	2.14446306	3.71809459	0.66985297
C	2.81948334	3.53170876	-0.57795116
C	2.05755242	3.39102861	-1.77157840
C	2.72297439	2.48075333	-2.63880595
C	1.96204440	1.63185090	-3.49292302
C	2.52985979	0.36313964	-3.77781051
C	1.68764916	-0.76765401	-3.97403380
C	2.32783278	-1.91646175	-3.41684710
C	1.55407029	-2.92965209	-2.78988742
C	2.16532662	-3.62487786	-1.71349664
C	1.37853486	-4.11754349	-0.62911709
C	2.13542557	-3.99391259	0.57585298
C	1.48575242	-3.67923571	1.79582883
C	2.22965620	-2.92034329	2.73980652
C	1.56733900	-1.99642765	3.60631785
C	2.41496522	-0.86572018	3.79899752
C	1.85192627	0.42459664	3.93099636
C	2.63209175	1.51170257	3.43310873
C	1.99124199	2.66369537	2.88097946
C	2.77727601	3.15165433	1.80310793
C	0.72211640	3.95510151	0.68508706
C	-0.04311712	3.62279056	1.88363138
C	0.59043621	2.83846192	2.92703341
C	-0.17420789	1.85617396	3.68256836
C	0.41693869	0.57155030	4.03355727
C	-0.42579462	-0.61694309	4.02574429
C	0.16612515	-1.89744998	3.66102527
C	-0.59661807	-2.87084470	2.89242254
C	0.03908799	-3.64350008	1.84181480
C	-0.72348482	-3.96198719	0.63775659
C	-0.02389904	-4.05200770	-0.63940368
C	-0.65457504	-3.57400198	-1.85718859
C	0.11024328	-2.86716293	-2.86570176
C	-0.52523767	-1.77986935	-3.60909732
C	0.28356004	-0.64801785	-4.03339890
C	-0.27465164	0.69445643	-4.02624749

C	0.53318167	1.82131938	-3.58689189
C	-0.10395093	2.90002486	-2.83261199
C	0.65850933	3.59503290	-1.81426995
C	0.02532031	4.05948344	-0.59257039
C	-1.37708613	4.12487046	-0.58474078
C	-2.13667390	3.98759940	0.61703122
C	-1.48972561	3.65911585	1.83478285
C	-2.23587175	2.88967530	2.76849308
C	-1.57539428	1.95583913	3.62588023
C	-2.42325736	0.82295615	3.80337699
C	-1.86040640	-0.46866431	3.92156492
C	-2.63938333	-1.54970919	3.40860039
C	-1.99734475	-2.69503201	2.84460054
C	-2.78136349	-3.17126239	1.76010836
C	-2.14581555	-3.72504149	0.62182324
C	-2.81828215	-3.52531925	-0.62507045
C	-2.05380954	-3.37109643	-1.81541591
C	-2.71695123	-2.45013111	-2.67320509
C	-1.95439560	-1.59142464	-3.51598692
C	-2.52146738	-0.31942334	-3.78728680
C	-1.67869962	0.81352524	-3.96859013
C	-2.32014248	1.95586313	-3.39975401
C	-1.54793188	2.96169745	-2.75945861
C	-2.16149657	3.64455794	-1.67645462
C	-3.44489135	3.24437469	-1.15486395
C	-3.42715202	3.45971770	0.27105965
C	-4.10734106	2.58572591	1.16150846
C	-3.52471013	2.34764135	2.43381714
C	-3.65154834	1.06480821	3.08375825
C	-4.36617805	-0.00499926	2.48558528
C	-3.85961814	-1.32371297	2.68958310
C	-3.96860613	-2.33564380	1.65058687
C	-4.65465323	-2.11767144	0.40461171
C	-4.02593068	-2.72521372	-0.75002662
C	-3.95090523	-2.04594337	-2.04431270
C	-4.47024297	-0.71740958	-2.24395146
C	-3.73095773	0.12648279	-3.12187033
C	-3.59734110	1.54762396	-2.89040336
C	-4.15223797	2.15797003	-1.73111572
C	-4.91557145	1.30694151	-0.84446163
C	-4.87875265	1.51417801	0.57696085
C	-5.05008209	0.24384860	1.22897402
C	-5.23729531	-0.78461832	0.20393389
C	-5.13532528	-0.09995291	-1.10155826

C	4.02773374	2.73433052	-0.70981272
C	3.95683759	2.07036259	-2.01258498
C	4.47754928	0.74405430	-2.22686217
C	3.73797968	-0.09019155	-3.11439569
C	3.60374619	-1.51412753	-2.89979296
C	4.15650961	-2.13792010	-1.74657281
C	3.44764127	-3.23061760	-1.18437474
C	3.42653354	-3.46204096	0.23899675
C	4.10468134	-2.59812731	1.14086893
C	3.51943519	-2.37454602	2.41453135
C	3.64482128	-1.09950184	3.07972102
C	4.35975159	-0.02262755	2.49473572
C	3.85309423	1.29331042	2.71324878
C	3.96388403	2.31642053	1.68602969
C	4.65192594	2.11233211	0.43957082
C	5.23599404	0.78244031	0.22443636
C	5.13974948	0.11303969	-1.08968236
C	4.91857642	-1.29709081	-0.84889090
C	4.87722949	-1.52015759	0.56999431
C	5.04549325	-0.25713696	1.23660511
La	2.77514037	0.47027000	-0.10737791
La	-2.77511669	-0.47173889	-0.10099475

$Y_2@D_5(285913)$-C_{100}

xyz file：

C	-1.85261078	-0.39808282	3.94646093
C	-2.62562611	-1.49589147	3.46155212
C	-1.97661147	-2.65043258	2.92102129
C	-2.75381012	-3.14532754	1.84261060
C	-2.11780847	-3.71430723	0.71783527
C	-2.79459420	-3.53445772	-0.52973518
C	-2.03037145	-3.40064006	-1.72074843
C	-2.70392338	-2.51127252	-2.59853804
C	-1.94570128	-1.67315700	-3.46423728
C	-2.52086777	-0.41276862	-3.76250182
C	-1.68826102	0.71977659	-3.97474623
C	-2.33578333	1.87056376	-3.42888525
C	-1.56947836	2.89507862	-2.81010910
C	-2.18441336	3.59532837	-1.74042821
C	-1.40249484	4.10433599	-0.65951607
C	-2.16004471	3.98783888	0.54635540

C	-1.51037544	3.68688484	1.77013246
C	-2.24981672	2.93370862	2.72117115
C	-1.58219625	2.02180274	3.59792832
C	-2.42268362	0.88727709	3.79942574
C	-0.41724724	-0.53392421	4.05204241
C	0.41759688	0.65893040	4.03372324
C	-0.18183364	1.93315175	3.65692115
C	0.57610655	2.90450618	2.87993497
C	-0.06378812	3.66004003	1.81862303
C	0.69685849	3.96958522	0.61284851
C	-0.00092475	4.04400504	-0.66635734
C	0.63240024	3.55275811	-1.87682844
C	-0.12527522	2.83779673	-2.88221942
C	0.51701045	1.74708906	-3.61455452
C	-0.28322254	0.60704682	-4.03202786
C	0.28286207	-0.73146633	-4.01163294
C	-0.51736606	-1.85824807	-3.55943250
C	0.12502071	-2.92572932	-2.79362727
C	-0.63261205	-3.60923202	-1.76653911
C	0.00084387	-4.06249340	-0.54138085
C	-0.69678506	-3.94835038	0.73492626
C	0.06392908	-3.60205874	1.93058500
C	-0.57582280	-2.81408488	2.96813899
C	0.18215973	-1.81909170	3.71450927
C	1.58245810	-1.90961876	3.65833855
C	2.42301036	-0.76947999	3.82488479
C	1.85298060	0.51985070	3.93228143
C	2.62603070	1.60218812	3.41367059
C	1.97691744	2.73948309	2.83777656
C	2.75403985	3.20087125	1.74457643
C	2.11795058	3.73503334	0.60286007
C	2.79452904	3.51633094	-0.63865794
C	2.03011197	3.34557701	-1.82472773
C	2.70358022	2.42962682	-2.67479821
C	1.94529520	1.56514928	-3.51402899
C	2.52050842	0.29630736	-3.77363123
C	1.68796322	-0.84232246	-3.95107396
C	2.33555292	-1.97571553	-3.36991344
C	1.56927395	-2.98065733	-2.71973033
C	2.18425829	-3.64743148	-1.62887794
C	1.40239969	-4.12261145	-0.53269037
C	2.16007033	-3.96897970	0.66896225
C	1.51049302	-3.63040893	1.88288226
C	2.24996059	-2.84819544	2.81015585

C	3.53307220	-2.29919860	2.47015455
C	3.65102345	-1.01043085	3.10759928
C	4.34664333	0.05884974	2.49299695
C	3.83809634	1.37249366	2.69013124
C	3.93854057	2.36272067	1.63353859
C	4.64507745	2.15167816	0.40178141
C	4.02230891	2.75011065	-0.76289892
C	3.95544737	2.05720025	-2.05320635
C	4.48480474	0.72801927	-2.24145007
C	3.72938682	-0.13165676	-3.09438204
C	3.60389798	-1.55266772	-2.85808231
C	4.16026882	-2.14601864	-1.69291678
C	3.46402656	-3.23275233	-1.10851574
C	3.44477985	-3.43400917	0.31878224
C	4.11240207	-2.54218335	1.19912286
C	4.85997270	-1.46491570	0.60065522
C	5.02098638	-0.18900304	1.23473923
C	5.24655355	0.82664992	0.21035930
C	5.15997162	0.12806221	-1.09383438
C	4.91150493	-1.27340372	-0.81813184
C	-3.83783553	-1.28874050	2.73144594
C	-3.93833450	-2.31113869	1.70589625
C	-4.64499907	-2.13828907	0.46832218
C	-4.02238908	-2.77244669	-0.67739266
C	-3.95569597	-2.11971435	-1.98849706
C	-4.48506506	-0.79694620	-2.21758091
C	-3.72961801	0.03597755	-3.09657182
C	-3.60419518	1.46363870	-2.90435144
C	-4.16051686	2.09277103	-1.75805309
C	-3.46420481	3.19704961	-1.20752712
C	-3.44479021	3.44230858	0.21286124
C	-4.11229961	2.57803515	1.12034803
C	-3.53296807	2.37450211	2.39831249
C	-3.65074870	1.10594637	3.07510909
C	-4.34642567	0.01820638	2.49393053
C	-5.02078005	0.22702504	1.22866489
C	-5.24639845	-0.81979999	0.23615976
C	-5.16007520	-0.16181194	-1.08899232
C	-4.91155242	1.24751106	-0.85665547
C	-4.85984296	1.48273410	0.55550987
Y	-2.96704931	-0.58418588	-0.23019631
Y	2.96707198	0.57682465	-0.24800980

$Sc_2@D_5$(285913)-C_{100}

xyz file：

C	-1.83921853	3.84076271	0.98800357
C	-2.58284517	3.20862114	2.02919824
C	-1.90169477	2.51188890	3.08000624
C	-2.66369672	1.37135184	3.43654533
C	-2.01543330	0.18143119	3.82903344
C	-2.69371509	-1.02958982	3.49445212
C	-1.93773461	-2.19198382	3.18433940
C	-2.63247117	-2.93624764	2.19673872
C	-1.89908668	-3.67347659	1.22906371
C	-2.50761677	-3.79473469	-0.04528709
C	-1.70726427	-3.84863091	-1.21716175
C	-2.38603913	-3.15395134	-2.26643479
C	-1.64732434	-2.39743967	-3.21612075
C	-2.28000469	-1.24428467	-3.74585064
C	-1.51145487	-0.10063286	-4.12099233
C	-2.26487383	1.07509532	-3.81702520
C	-1.60719055	2.24686656	-3.36559671
C	-2.32541218	3.08251278	-2.46942323
C	-1.63317675	3.82950010	-1.46327715
C	-2.44300808	3.87044097	-0.28989199
C	-0.40108099	3.93080437	1.09816262
C	0.40056617	4.07986966	-0.10636964
C	-0.23280186	3.88019367	-1.40473732
C	0.49938430	3.24673829	-2.49418357
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C	-0.20218579	-2.47227438	-3.20817452
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C	-0.58934007	0.17090932	4.02871251
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C	2.44235440	3.68223183	1.22487333

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C	1.90157553	3.18765397	-2.37449387
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C	2.01533212	1.11015478	-3.66887165
C	2.69380051	-0.14583890	-3.63941049
C	1.93788605	-1.34873115	-3.62210228
C	2.63281433	-2.31150917	-2.84600792
C	1.89938001	-3.26224278	-2.08711290
C	2.50809216	-3.69120059	-0.88120686
C	1.70792955	-4.02992029	0.24219986
C	2.38664324	-3.61158738	1.42921044
C	1.64773721	-3.10929256	2.53447737
C	2.28023244	-2.11983829	3.32913972
C	1.51149224	-1.10235875	3.97141899
C	2.26493276	0.11187600	3.96407413
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C	2.32507955	2.38720334	3.14656642
C	3.59139854	2.13160602	2.52207275
C	3.67490366	2.94206651	1.33111685
C	4.33599601	2.48329908	0.16863446
C	3.79552687	2.86251266	-1.08900944
C	3.86204092	1.94469253	-2.21003652
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C	3.89039218	-1.73825088	-2.41709902
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C	3.72536794	-3.07183795	-0.39547387
C	3.64084322	-3.04229238	1.04796691
C	4.21200080	-1.96774208	1.77997320
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C	4.88230483	0.39805779	1.39870778
C	5.00224027	1.19936359	0.21785804
C	5.22415417	0.33064664	-0.93140058
C	5.16616872	-1.05945504	-0.41975464
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C	-3.59138288	2.68195260	-1.92589884
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$La_2C_2@C_1$(230933)-C_{98}

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C	1.08119095	4.45872492	1.40244530
C	4.21147898	0.54352085	1.69611710
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C	1.42970914	3.60930677	2.50645540
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C	2.66525795	-3.35918766	2.24551762
C	3.42290660	-2.15275834	2.25308934
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C	1.78409198	-1.24980166	3.87058037
C	-2.14848810	3.47259437	2.54512097
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C	-1.01146479	-4.51782144	-0.14639597
C	0.39525116	-4.56583927	-0.26350391
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C	-1.23786290	-3.41163317	-2.33433021
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C	-4.61024264	-1.66145682	-0.45834365
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C	-3.35845182	-2.05769365	-2.53993105
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C	-3.38576162	-2.51069252	1.60729704
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C	0.45848072	-4.21660806	2.19826372
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C	4.16134283	0.61184941	1.68270337
C	3.24008916	0.39410388	2.76551849
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C	2.45108808	2.75552238	2.41276406
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C	0.87411589	-0.16801885	4.16610344
C	1.10598236	1.16270582	3.80480985
C	2.70879693	-3.30884482	2.25540701
C	3.44371442	-2.08926220	2.26092141
C	2.95294479	-0.98518596	3.09895976
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C	-2.21359621	3.44773018	2.51880605
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C	-0.94441402	3.98210134	2.49945906
C	-0.06192095	2.02769269	3.73471817
C	0.12347930	3.29368305	3.16257560
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C	-0.64661184	0.44892799	0.39623388
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C	3.95371740	2.39955092	-1.54673520
C	3.06781395	3.44691314	-1.20439891
C	4.58909177	1.69565856	-0.44526358
C	3.86834450	0.16774512	-2.75189373
C	4.18277099	-1.87081344	-1.44891000
C	4.54363539	-0.52405794	-1.67399775
C	4.87993679	0.27266396	-0.51014279
C	-1.37589202	-1.38885615	-3.68554946
C	0.00993538	-1.13576620	-3.75203889
C	0.91462046	-2.16097406	-3.23977894

C	2.30862158	-1.81639273	-3.09142352
C	2.72493899	-0.47552483	-3.36792449
C	3.13152884	-2.54375004	-2.20700211
C	4.61126485	-0.28565969	0.80020217
C	4.18955388	-2.46737935	-0.13110854
C	4.28274720	-1.65581882	1.03113294
C	3.30164691	-3.58617089	-0.16070830
C	-0.78057280	-4.56090778	-0.18726197
C	0.62608529	-4.53748303	-0.30222620
C	1.32986007	-4.51009608	0.93328929
C	2.67145297	-3.97676695	1.00578330
C	-1.90836563	-2.53929230	-3.03790906
C	-1.61767406	-4.12376330	-1.25332200
C	-1.05438041	-3.46091684	-2.37581313
C	0.38770054	-3.29700445	-2.48936334
C	1.22753132	-3.95839355	-1.50689299
C	2.59546463	-3.59464797	-1.42094883
C	-4.52965160	-1.89887467	-0.50968070
C	-2.86562689	-3.68111614	-0.68448473
C	-3.72633510	-2.76639861	-1.34120207
C	-3.24151428	-2.21988361	-2.58353197
C	-0.29536048	-2.14505272	3.84113661
C	-1.24300258	-2.83829717	3.04711291
C	-2.46477655	-2.14687287	2.69313306
C	-2.71034729	-3.71210243	0.76251570
C	-3.23682880	-2.67147110	1.55918679
C	-4.19359690	-1.83044726	0.90527945
C	0.66611842	-4.18970333	2.16261651
C	1.59831166	-3.40855144	2.94388969
C	1.11982171	-2.41020204	3.74861143
C	-1.44778674	-4.29281699	1.05406774
C	-0.72652035	-3.92736326	2.21384132
Sc	-2.58077720	-0.73077501	-0.76283265
Sc	2.56171568	0.62026140	-0.85751237
C	-0.63957969	-0.11499753	-0.11615357
C	0.58348398	0.13852688	-0.17675945

Table S4 Relative energies (in kcal/mol) of two different electronic states of some important isomers at B3LYP/6-31G(d) ~ Lanl2dz level.

B3LYP/6-31G(d) ~ Lanl2dz	singlet state	ΔE(kcal/mol) of triplet state
Sc_2C_2@ C_1(230933)-C_{98}	0	14.9
Sc_2@ D_5(285913)-C_{100}	0	19.5
Y_2C_2@ C_1(230933)-C_{98}	0	15.4
La_2C_2@ C_1(230933)-C_{98}	0	15.4

Table S5 Relative energies (in kcal/mol) and HOMO-LUMO gaps (in eV) of $La_2C_2@C_1(230933)$-C_{98} and $La_2@\ D_5(285913)$-C_{100}, obtained on the levels of B3LYP/6-31G(d) ~ Lanl2dz and M06-2X/6-31G(d) ~ Lanl2dz, respectively.

	B3LYP/6-31G(d) ~ Lanl2dz		M06-2X/6-31G(d) ~ Lanl2dz	
	ΔE	Gap	ΔE	Gap
$La_2C_2@\ C_1(230933)$-C_{98}	34.6	1.48	22.3	2.75
$La_2@\ D_5(285913)$-C_{100}	0	1.54	0	2.36

Table S6 Relative energies (in kcal/mol) and HOMO-LUMO gaps (in eV) of $Y_2C_2@C_1(230933)$-C_{98} and $Y_2@\ D_5(285913)$-C_{100}, obtained on the levels of B3LYP/6-31G(d) ~ Lanl2dz and M06-2X/6-31G(d) ~ Lanl2dz, respectively.

	B3LYP/6-31G(d) ~ Lanl2dz		M06-2X/6-31G(d) ~ Lanl2dz	
	ΔE	Gap	ΔE	Gap
$Y_2C_2@\ C_1(230933)$-C_{98}	10.7	1.48	0.2	2.77
$Y_2@\ D_5(285913)$-C_{100}	0	1.54	0	2.25

Table S7 Relative energies (in kcal/mol) and HOMO-LUMO gaps (in eV) of $Sc_2C_2@C_1(230933)$-C_{98} and $Sc_2@D_5(285913)$-C_{100}, obtained on the levels of B3LYP/6-31G(d) ~ Lanl2dz and M06-2X/6-31G(d) ~ Lanl2dz, respectively.

	B3LYP/6-31G(d) ~ Lanl2dz		M06-2X/6-31G(d) ~ Lanl2dz	
	ΔE	Gap	ΔE	Gap
$Sc_2C_2@C_1(230933)$-C_{98}	0.9	0.90	-8.8	2.73
$Sc_2@D_5(285913)$-C_{100}	0	1.85	0	2.59

Table S8 NBO analysis of the two inside carbon atoms in cages*.

	Occupancy/ Bond orbital	Hybrids
La_2C_2@ C_1(23093 3)-C_{98}	1.91619/ BD (1)	(49.72%) 0.7051* C 101 s(45.30%)p 1.21(54.62%)d 0.00(0.07%) -0.0015 0.6702 0.0619 -0.1394 -0.0085 0.6679 0.0744 0.2736 0.0170 -0.0071 -0.0020 0.0100 -0.0174 -0.0165 (50.28%) 0.7091* C 102 s(46.15%)p 1.17(53.79%)d 0.00(0.07%) -0.0017 0.6759 0.0675 0.1320 0.0100 -0.6904 -0.0779 0.1939 0.0042 -0.0068 0.0009 -0.0040 -0.0176 -0.0178
	1.84201/ BD (2)	(48.85%) 0.6989* C 101 s(0.01%)p99.99(99.77%)d 17.40(0.21%) -0.0002 -0.0108 -0.0027 0.9731 -0.0647 0.2157 -0.0101 -0.0030 -0.0005 0.0424 -0.0067 -0.0015 -0.0174 -0.0006 (51.15%) 0.7152* C 102 s(0.05%)p99.99(99.75%)d 4.38(0.20%) 0.0002 0.0215 0.0021 0.9749 -0.0652 0.2065 -0.0102 -0.0047 0.0014 -0.0403 -0.0123 -0.0023 0.0161 0.0004
	1.76403/ BD (3)	(49.16%) 0.7011* C 101 s(1.79%)p54.90(98.01%)d 0.11(0.20%) 0.0013 -0.1327 0.0155 0.0564 -0.0013 -0.2482 -0.0012 0.9566 -0.0153 0.0030 -0.0081 0.0438 0.0072 0.0016 (50.84%) 0.7130* C 102 s(1.62%)p60.56(98.18%)d 0.12(0.20%) 0.0015 -0.1261 0.0177 -0.0240 0.0001 0.1487 0.0038 0.9793 -0.0133 0.0006 0.0076 -0.0428 0.0025 -0.0076
Y_2C_2@ C_1(23093 3)-C_{98}	1.91634/ BD (1)	(50.37%) 0.7098* C 99 s(51.68%)p 0.93(48.26%)d 0.00(0.06%) 0.0017 -0.7170 -0.0523 0.4313 0.0337 -0.5070 -0.0636 -0.1841 -0.0213 0.0171 0.0055 -0.0067 0.0029 0.0146 (49.63%) 0.7045* C 100 s(49.41%)p 1.02(50.52%)d 0.00(0.06%) 0.0017 -0.7001 -0.0635 -0.4849 -0.0224 0.5125 0.0701 0.0451 0.0042 0.0186 0.0027 -0.0063 0.0047 0.0147

	1.87130/ BD (2)	(52.55%) 0.7249* C 99 s(2.11%)p46.35(97.74%)d 0.07(0.15%) -0.0007 -0.1451 -0.0050 0.6678 -0.0286 0.6689 -0.0099 0.2882 -0.0119 0.0084 -0.0055 0.0090 -0.0368 -0.0005 (47.45%) 0.6888* C 100 s(1.36%)p72.27(98.46%)d 0.13(0.18%) 0.0010 0.1128 0.0299 0.6201 -0.0080 0.7207 -0.0131 0.2834 0.0110 -0.0085 -0.0019 -0.0164 0.0383 -0.0006
	1.81170/ BD (3)	(51.96%) 0.7209* C 99 s(0.04%)p99.99(99.81%)d 4.20(0.15%) 0.0008 0.0150 0.0119 -0.0192 -0.0044 -0.3761 0.0047 0.9253 0.0084 0.0061 -0.0211 0.0293 0.0122 0.0074 (48.04%) 0.6931* C 100 s(0.12%)p99.99(99.70%)d 1.45(0.18%) 0.0002 -0.0352 -0.0002 -0.1323 0.0093 -0.2565 -0.0009 0.9558 -0.0015 -0.0017 0.0217 -0.0299 -0.0120 -0.0171
Sc_2C_2@ C_1(23093 3)-C_{98}	1.94767/ BD (1)	(50.03%) 0.7073* C 101 s(56.18%)p 0.78(43.77%)d 0.00(0.05%) -0.0010 0.7474 0.0565 0.6424 0.0746 0.1341 0.0158 -0.0336 0.0053 0.0077 -0.0021 -0.0002 0.0185 -0.0112 (49.97%) 0.7069* C 102 s(56.67%)p 0.76(43.27%)d 0.00(0.05%) -0.0010 0.7507 0.0566 -0.6426 -0.0756 -0.1046 -0.0131 0.0521 0.0144 0.0067 -0.0031 -0.0006 0.0188 -0.0112
	1.85121/ BD (2)	(50.54%) 0.7109* C 101 s(0.17%)p99.99(99.75%)d 0.51(0.08%) 0.0002 0.0391 0.0115 0.0058 0.0025 -0.0025 -0.0011 0.9986 0.0140 0.0000 0.0275 0.0033 0.0010 -0.0083 (49.46%) 0.7033* C 102 s(0.05%)p99.99(99.87%)d 1.59(0.08%) 0.0000 0.0224 0.0042 0.1047 0.0023 0.0161 0.0007 0.9936 0.0173 -0.0008 -0.0281 -0.0052 -0.0025 -0.0001
	1.83052/ BD (3)	(50.13%) 0.7080* C 101 s(0.01%)p 1.00(99.91%)d 0.00(0.08%) 0.0001 0.0065 0.0045 -0.2117 -0.0037 0.9767 0.0191 0.0034 -0.0011 0.0268

		0.0013 -0.0068 -0.0091 0.0012 (49.87%) 0.7062* C 102 s(0.02%)p99.99(99.89%)d 3.50(0.08%) -0.0001 -0.0147 -0.0043 -0.1775 -0.0025 0.9833 0.0210 0.0031 -0.0007 -0.0267 0.0003 -0.0015 0.0101 0.0000

*M-M bonding haven't been observed at $M_2@C_{100}$ and $M_2C_2@C_{98}$.

Figure S1 Corresponding energy orders of isomers of (a) La_2C_{100}, (b) Y_2C_{100} and (c) Sc_2C_{100}, obtained at the level of B3LYP/6-31G(d) ~ Lanl2dz. Squares indicate isomers of $M_2@C_{100}$ (M = La, Y, Sc), and circles indicate isomers of $M_2C_2@C_{98}$ (M= La, Y, Sc), respectively.

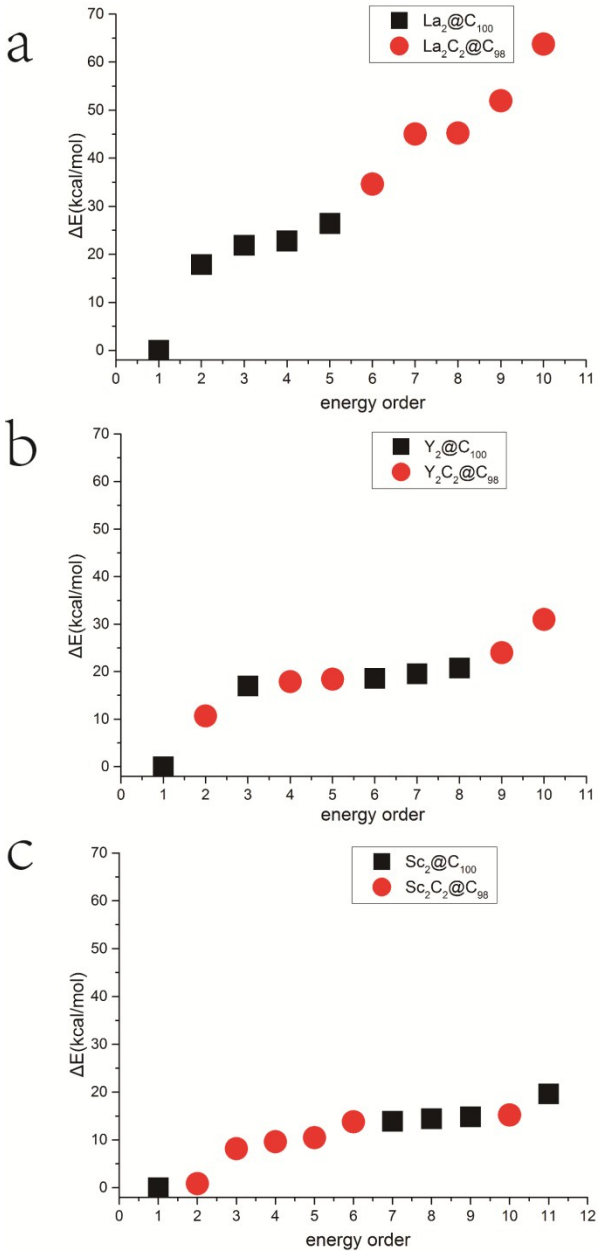
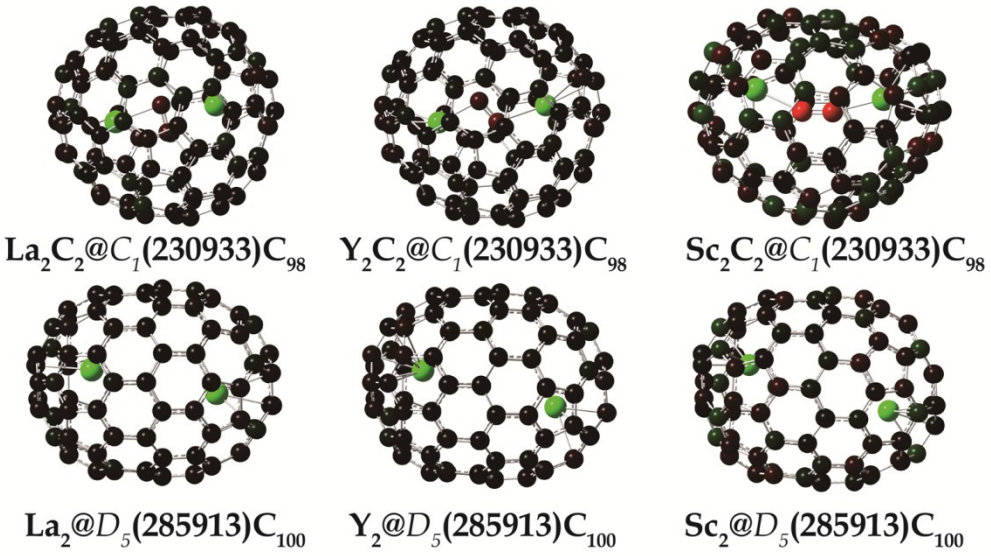
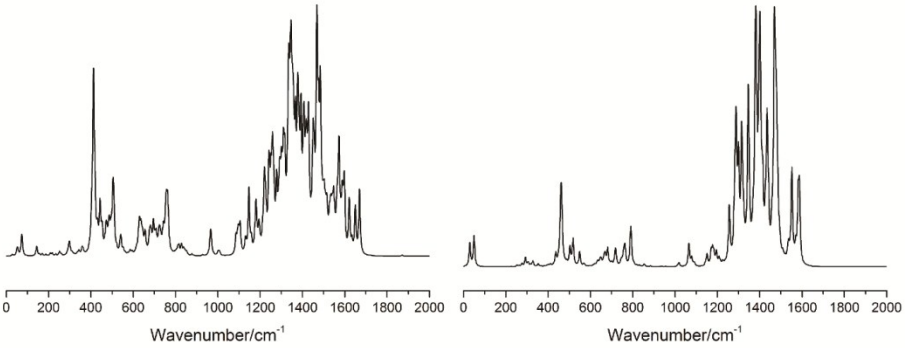


Figure S2 NBO charge distributions of the most sable isomers of M_2@C100 and M_2C_2@C_{98} (M= La, Y, Sc)*. Green represents positive charge and red represents negative charge.

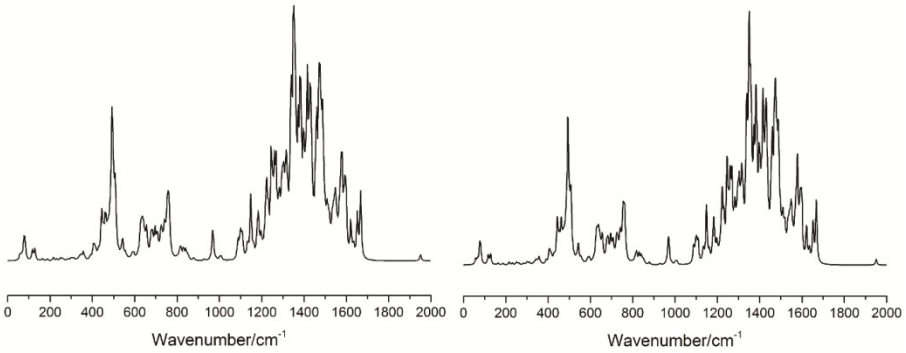


*The calculated at B3LYP/6-31G(d)_LANL2DZ level failed and B3LYP/6-31G(d)_SDD level is used here.

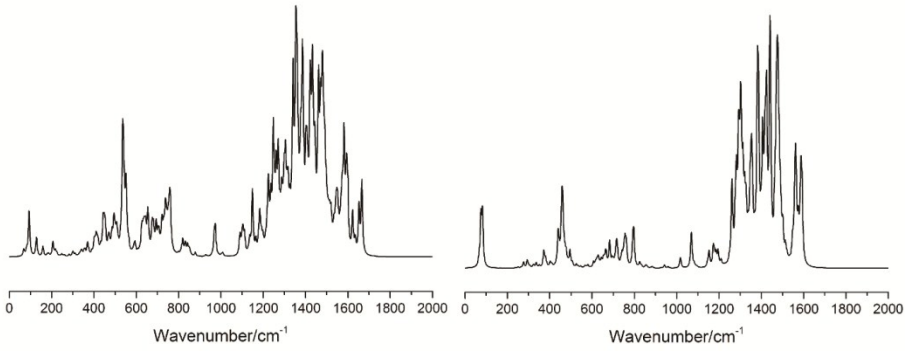
Figure S3 Simulated IR spectra of main M_2C_{100} isomers.



$La_2C_2@C_1(230933)C_{98}$ $La_2@D_5(285913)C_{100}$



$Y_2C_2@C_1(230933)C_{98}$ $Y_2@D_5(285913)C_{100}$



$Sc_2C_2@C_1(230933)C_{98}$ $Sc_2@D_5(285913)C_{100}$