Electronic Supplementary Information for

Probing the Role of Encapsulated Alkaline Earth Metal Atom in Endohedral Metallofullerenes $M@C_{76}$ (M=Ca, Sr, and Ba) by First-Principles Calculations

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Electronic Supplementary Material (ESI) for Dalton Transactions

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I. Optimized relative energies and HOMO-LUMO gaps of all selected M@C_{76} (M=Ca, Sr, and Ba) isomers.

As the alkaline earth metal transfers two electrons to the carbon cages, the energy order of M@C_{76} may in accordance with that of di-anions. The energy order of di-anions C_{76}^{2-} can be obtained in the Supporting Information of ref.37. We chose several most stable di-anions C_{76}^{2-} as the candidates of M@C_{76}, including two IPR, all PA=1 isomers and two PA=2 isomers. The molecular structures of endohedral fullerene M@C_{76} were optimized at B3LYP/6-31G(d)-Lanl2dz level. The calculated results of IPR, PA=1 and main PA=2 isomers have been collected in Table S1.

Table S1 Relative energies and HOMO-LUMO gaps of all selected M@C_{76} (M=Ca, Sr, and Ba) isomers.

C_{76} spiral ID	PA	sym.	Ca@C_{76}		Sr@C_{76}		Ba@C_{76}	
			ΔE	gap	ΔE	gap	ΔE	gap
			kcal/mol	eV	kcal/mol	eV	kcal/mol	eV
17459	1	C_1	0.00	1.71	0.00	1.70	0.00	1.68
19138	1	C_{2v}	0.39	1.42	0.61	1.41	0.28	1.40
19151	0	T_d	6.53	0.93	5.49	0.91	4.02	0.88
17646	1	C_2	6.95	1.88	7.05	1.87	7.43	1.87
17894	1	C_1	7.25	1.38	8.16	1.36	9.17	1.33
17418	1	C_1	11.21	1.25	10.70	1.26	10.30	1.27
17410	1	C_s	12.84	1.73	12.26	1.76	11.81	1.79
17750	1	C_1	13.59	1.21	14.16	1.16	14.91	1.10
19150	0	D_2	13.87	0.99	12.88	0.94	11.45	0.95
18632	1	C_1	15.43	1.47	15.75	1.44	15.93	1.40
18542	1	C_1	16.23	1.12	16.77	1.08	17.51	1.03
19142	1	C_s	16.94	1.19	16.46	1.24	13.86	1.31
18944	2	C_2	20.0	1.42	19.67	1.45	18.45	1.51
18439	1	C_1	23.87	1.51	24.1	1.46	25.41	1.41
18943	2	C_1	24.13	1.45	24.2	1.50	23.39	1.58
18720	1	C_1	32.00	1.13	32.5	1.09	33.31	1.06

II. Zero point energy of M@C_1(17459)-C_{76} and M@C_{2v}(19138)-C_{76} (M=Ca, Sr, and Ba) calculated at B3LYP/3-21G-Lanl2dz level of theory.

To further show the different performance of M@C_1(17459)-C_{76} and M@C_{2v}(19138)-C_{76} (M=Ca, Sr, and Ba) at 0K, the zero point energy of M@C_1(17459)-C_{76} and M@C_{2v}(19138)-C_{76} (M=Ca, Sr, and Ba) calculated at the B3LYP/3-21G-Lanl2dz level of theory has been collected in Table S2.

Table S2 Zero point energy of M@C_1(17459)-C_{76} and M@C_{2v}(19138)-C_{76} (M=Ca, Sr, and Ba) at B3LYP/3-21G-Lanl2dz level of theory.

C_{76}	Energy ΔE kcal/mol	zero point energy(ZPE) E kcal/mol	ZPE corrected energy ΔE kcal/mol
Ca@C_1(17459)	0.00	292.37	0.00
Ca@C_{2v}(19138)	2.08	291.98	1.69
Sr@C_1(17459)	0.00	292.25	0.00
Sr@C_{2v}(19138)	2.54	291.90	2.19
Ba@C_1(17459)	0.00	292.28	0.00
Ba@C_{2v}(19138)	2.39	291.89	1.99

It's notably that these energies are obtained at the B3LYP/3-21G-Lanl2dz level of theory. On the other hand, the relative energies provided in the paper are calculated at the B3LYP/6-31G(d)-Lanl2dz level of theory, which are always viewed much more precise. Thus, the relative energies have a few differences. In Table S2, it's obvious that even though the encapsulated metal changes, the zero point energy for M@C_1(17459) is little smaller than that for M@C_{2v}(19138), which reduces the energy difference between M@C_1(17459) and M@C_{2v}(19138).

III. Cartesian coordinates of molecular structures of M@C_1(17459)-C_{76} and M@C_{2v}(19138)-C_{76} (M=Ca, Sr, and Ba).

A. Ca@C_1(17459)-C_{76}.

Coordinates:

C	-0.016096	-0.064872	0.110891
C	1.370518	-0.056216	0.110248
C	2.106736	1.186620	0.105207

C	3.296231	0.977445	-0.673159
C	3.935222	2.044493	-1.353006
C	4.583941	1.739500	-2.589549
C	4.725726	2.727580	-3.625652
C	4.654679	2.047859	-4.892933
C	4.165573	2.696816	-6.077990
C	3.410188	1.866669	-6.980410
C	2.211194	2.390559	-7.620238
C	1.201050	1.353525	-7.611471
C	-0.153210	1.597862	-7.237102
C	-0.921626	0.496809	-6.638850
C	-2.025831	0.791500	-5.718684
C	-2.402041	-0.161155	-4.725155
C	-2.797432	0.239078	-3.402999
C	-2.350130	-0.783816	-2.467016
C	-1.895686	-0.421370	-1.206780
C	-0.734600	-1.068450	-0.637273
C	-0.727130	1.201658	0.000725
C	-1.878917	0.983572	-0.818746
C	-2.366752	1.994131	-1.692959
C	-2.837794	1.604103	-3.031015
C	-2.707970	2.541571	-4.095501
C	-2.302091	2.147115	-5.405085
C	-1.553813	3.233911	-6.006074
C	-0.510692	2.995837	-6.935580
C	0.477532	4.030546	-7.058172
C	1.845559	3.731946	-7.458164
C	2.730162	4.618861	-6.758769
C	3.813160	4.096386	-5.972540
C	3.725675	4.724099	-4.656172
C	4.166144	4.040748	-3.472768
C	3.489981	4.338197	-2.250224
C	3.387435	3.350585	-1.187307
C	2.154368	3.535944	-0.491965
C	1.439086	2.440924	0.082965
C	-0.029534	2.444669	0.000324
C	-0.673757	3.513430	-0.687408
C	-1.806145	3.290151	-1.519020
C	-1.725317	4.238942	-2.624554
C	-2.182045	3.867382	-3.873156
C	-1.466608	4.297438	-5.044991
C	-0.320510	5.145084	-4.956895
C	0.556782	5.115377	-6.084345
C	1.936187	5.480952	-5.938408

C	2.514699	5.534826	-4.634658
C	1.677843	5.577101	-3.464577
C	2.271903	5.096874	-2.253878
C	1.466568	4.615643	-1.157582
C	0.088895	4.612038	-1.272282
C	-0.541229	5.047129	-2.486388
C	0.221543	5.462382	-3.621011
C	2.096540	-1.014397	-0.704011
C	3.249756	-0.358127	-1.242773
C	3.665143	-0.587353	-2.580745
C	4.412271	0.458060	-3.203450
C	4.416314	0.649335	-4.622315
C	3.609868	-0.152066	-5.477047
C	3.167853	0.468500	-6.684360
C	1.862606	0.147599	-7.193307
C	1.136445	-0.889738	-6.656374
C	-0.281160	-0.763760	-6.486534
C	-0.657227	-1.702606	-5.451003
C	-1.720123	-1.432742	-4.610380
C	-1.668799	-1.816206	-3.213159
C	-0.513515	-2.406855	-2.692083
C	-0.032071	-2.026083	-1.387191
C	1.412708	-1.961712	-1.453874
C	1.829498	-2.224922	-2.820104
C	2.895724	-1.506097	-3.429112
C	2.833786	-1.257571	-4.879461
C	1.678162	-1.689838	-5.576534
C	0.559261	-2.285535	-4.904479
C	0.642193	-2.587971	-3.555894
Ca	1.707673	2.848063	-4.781794

B. Ca@C_{2v}(19138)-C_{76}.

Coordinates:

C	0.898327	-0.709801	-3.696581
C	-0.501340	-1.141764	-3.695893
C	1.909657	-1.464181	-3.033301
C	1.520783	-2.691970	-2.319280
C	0.144456	-3.092962	-2.355797
C	-0.849698	-2.310931	-3.052305
C	-1.901629	-3.250193	-1.225061
C	-2.105431	-2.382390	-2.342788

C	-0.503224	-3.661430	-1.224918
C	-0.499178	1.141970	-3.695480
C	-1.368326	0.000920	-3.667352
C	0.899666	0.707356	-3.696321
C	-3.014164	-1.267677	-2.299143
C	-2.596086	0.001946	-2.919016
C	-3.912613	-1.237230	-1.176958
C	-3.646981	-2.057907	-0.000342
C	-2.602096	-3.033415	-0.000459
C	-4.454072	0.003050	0.717622
C	-4.454075	0.003306	-0.717669
C	-3.912601	-1.237599	1.176494
C	-3.011774	1.272144	-2.298702
C	-3.910258	1.242980	-1.176516
C	0.150305	3.091475	-2.354690
C	-0.845325	2.311560	-3.051469
C	1.525864	2.687849	-2.318312
C	1.912413	1.459585	-3.032770
C	-2.100914	2.385134	-2.341923
C	-1.895490	3.252181	-1.223907
C	-0.496304	3.660763	-1.223610
C	-3.643070	2.062724	0.000392
C	-2.596350	3.036271	0.000624
C	3.030541	0.712492	-2.568927
C	3.029191	-0.719356	-2.569185
C	3.811094	1.154080	-1.418796
C	3.402945	2.284470	-0.723227
C	2.266715	3.060066	-1.171240
C	3.808905	-1.162817	-1.419205
C	4.280947	-0.004939	-0.704698
C	-3.910241	1.242507	1.176936
C	-3.011864	1.271273	2.299184
C	-2.596252	0.000905	2.919103
C	-3.014258	-1.268447	2.298721
C	-1.901750	-3.250653	1.224117
C	-2.105620	-2.383217	2.342116
C	-0.845593	2.310469	3.052591
C	-2.101107	2.384297	2.342958
C	-0.499500	1.140657	3.696225
C	-1.368636	-0.000385	3.667628
C	-1.895610	3.251766	1.225281
C	-0.849966	-2.312011	3.051775
C	0.144251	-3.093783	2.355059
C	-0.503335	-3.661866	1.223932

C	0.203572	-3.859565	-0.000495
C	-0.501663	-1.143083	3.695823
C	0.898004	-0.711119	3.696760
C	1.909391	-1.465259	3.033304
C	1.520576	-2.692790	2.318806
C	0.899343	0.706039	3.697007
C	-0.496416	3.660328	1.225238
C	0.150100	3.090622	2.356161
C	1.912148	1.458501	3.033820
C	1.525661	2.687023	2.319765
C	3.398551	-2.292936	0.723882
C	2.260836	-3.066412	1.171803
C	3.398615	-2.292675	-0.724043
C	2.260935	-3.065986	-1.172339
C	1.598780	-3.586739	-0.000387
C	3.808778	-1.163323	1.419483
C	3.028970	-0.720270	2.569559
C	3.030318	0.711575	2.569810
C	3.810964	1.153572	1.419898
C	4.280880	-0.005191	0.705426
C	3.402882	2.284214	0.724700
C	2.266620	3.059659	1.172893
C	1.605542	3.581647	0.000894
C	0.210860	3.857136	0.000883
Ca	-1.743678	0.000468	-0.001114

C. Sr@*C*$_1$(17459)-C$_{76}$.

Coordinates:

C	-0.015203	-0.062627	0.109004
C	1.371765	-0.053403	0.107785
C	2.107433	1.189516	0.102637
C	3.296980	0.980540	-0.677020
C	3.934596	2.047954	-1.358005
C	4.583633	1.744796	-2.595425
C	4.733495	2.732473	-3.631393
C	4.665490	2.050497	-4.898686
C	4.167293	2.698328	-6.081240
C	3.411836	1.869837	-6.983582
C	2.211953	2.391661	-7.622271
C	1.201804	1.355899	-7.615896
C	-0.152965	1.601075	-7.243309

C	-0.920254	0.499781	-6.642558
C	-2.024079	0.793976	-5.720552
C	-2.400796	-0.158867	-4.727148
C	-2.797272	0.241081	-3.404591
C	-2.349006	-0.781680	-2.468994
C	-1.895002	-0.419647	-1.208294
C	-0.733632	-1.066402	-0.639079
C	-0.726378	1.203742	-0.001030
C	-1.878522	0.985455	-0.820391
C	-2.366121	1.996077	-1.694819
C	-2.837039	1.605927	-3.032751
C	-2.707811	2.544132	-4.097206
C	-2.299624	2.150105	-5.406702
C	-1.552789	3.237650	-6.008829
C	-0.510363	2.999733	-6.941010
C	0.476611	4.031162	-7.059366
C	1.843716	3.728889	-7.452412
C	2.726064	4.611605	-6.751923
C	3.807772	4.092826	-5.969195
C	3.727200	4.727088	-4.657198
C	4.172239	4.047215	-3.477473
C	3.490967	4.341918	-2.255042
C	3.387498	3.354595	-1.192163
C	2.154643	3.539910	-0.494733
C	1.439528	2.443906	0.079968
C	-0.028943	2.447222	-0.002105
C	-0.673524	3.516282	-0.689633
C	-1.806003	3.292658	-1.521093
C	-1.724789	4.241868	-2.627125
C	-2.181592	3.869673	-3.875483
C	-1.466011	4.300808	-5.048061
C	-0.321233	5.151350	-4.959506
C	0.557048	5.114066	-6.083730
C	1.934561	5.475661	-5.935150
C	2.514617	5.535526	-4.635132
C	1.677929	5.585533	-3.467070
C	2.272427	5.101722	-2.257401
C	1.467199	4.619335	-1.160821
C	0.088973	4.615325	-1.275464
C	-0.540620	5.050786	-2.489568
C	0.221604	5.470644	-3.624612
C	2.097804	-1.011532	-0.706783
C	3.251081	-0.355219	-1.245671
C	3.665045	-0.583460	-2.584726

C	4.410828	0.462370	-3.208470
C	4.421502	0.652722	-4.627984
C	3.612780	-0.149624	-5.482102
C	3.169641	0.471045	-6.688598
C	1.863334	0.149479	-7.196972
C	1.137318	-0.887851	-6.660156
C	-0.280761	-0.761674	-6.490087
C	-0.656481	-1.700161	-5.453662
C	-1.719481	-1.430877	-4.612733
C	-1.667763	-1.814103	-3.215339
C	-0.512500	-2.404989	-2.694142
C	-0.030959	-2.024161	-1.389240
C	1.413784	-1.958924	-1.456523
C	1.830326	-2.222646	-2.823000
C	2.896304	-1.503129	-3.432589
C	2.835006	-1.254300	-4.883050
C	1.678875	-1.687626	-5.579762
C	0.560066	-2.283098	-4.907133
C	0.643154	-2.586077	-3.558465
Sr	1.644326	2.656620	-4.584048

D. Sr@C_{2v}(19138)-C_{76}.

Coordinates:

C	0.894816	-0.709879	-3.697573
C	-0.505914	-1.141394	-3.697160
C	1.906258	-1.464045	-3.033719
C	1.517196	-2.691588	-2.319735
C	0.140754	-3.092665	-2.357364
C	-0.853989	-2.311042	-3.053649
C	-1.907011	-3.248914	-1.225853
C	-2.110945	-2.382120	-2.344884
C	-0.508140	-3.658455	-1.224859
C	-0.503754	1.141610	-3.696750
C	-1.373833	0.000926	-3.668808
C	0.896155	0.707439	-3.697313
C	-3.020908	-1.267833	-2.304184
C	-2.605844	0.001959	-2.924553
C	-3.908832	-1.236104	-1.175944
C	-3.649556	-2.058705	-0.000426
C	-2.608329	-3.033427	-0.000564
C	-4.444549	0.003040	0.716020

C	-4.444410	0.003296	-0.716188
C	-3.909092	-1.236587	1.175434
C	-3.018533	1.272318	-2.303747
C	-3.906508	1.241853	-1.175509
C	0.146596	3.091182	-2.356257
C	-0.849621	2.311682	-3.052818
C	1.522272	2.687471	-2.318769
C	1.909012	1.459450	-3.033190
C	-2.106439	2.384875	-2.344024
C	-1.900883	3.250906	-1.224698
C	-0.501233	3.657787	-1.223550
C	-3.645673	2.063536	0.000309
C	-2.602602	3.036299	0.000519
C	3.027690	0.712663	-2.569362
C	3.026344	-0.719527	-2.569622
C	3.808325	1.154100	-1.419052
C	3.399749	2.284593	-0.723368
C	2.263893	3.060360	-1.171869
C	3.806139	-1.162839	-1.419462
C	4.278286	-0.004940	-0.704998
C	-3.906763	1.241497	1.175883
C	-3.018938	1.271566	2.304317
C	-2.606279	0.000916	2.924729
C	-3.021319	-1.268725	2.303851
C	-1.907119	-3.249305	1.224745
C	-2.111204	-2.382957	2.344093
C	-0.849908	2.310597	3.053801
C	-2.106700	2.384048	2.344939
C	-0.504091	1.140290	3.697347
C	-1.374180	-0.000380	3.668907
C	-1.900990	3.250424	1.225908
C	-0.854276	-2.312129	3.052979
C	0.140529	-3.093514	2.356531
C	-0.508252	-3.658869	1.223746
C	0.199396	-3.856160	-0.000561
C	-0.506251	-1.142707	3.696941
C	0.894482	-0.711197	3.697669
C	1.905988	-1.465134	3.033634
C	1.516988	-2.692416	2.319175
C	0.895820	0.706121	3.697916
C	-0.501346	3.657333	1.225050
C	0.146373	3.090356	2.357635
C	1.908742	1.458377	3.034152
C	1.522068	2.686651	2.320136

C	3.395359	-2.293056	0.723941
C	2.258001	-3.066686	1.172339
C	3.395424	-2.292802	-0.724185
C	2.258118	-3.066285	-1.172969
C	1.595054	-3.585606	-0.000444
C	3.806025	-1.163348	1.419668
C	3.026113	-0.720447	2.569904
C	3.027458	0.711752	2.570152
C	3.808209	1.153595	1.420082
C	4.278235	-0.005192	0.705663
C	3.399685	2.284331	0.724758
C	2.263780	3.059930	1.173430
C	1.601807	3.580509	0.000837
C	0.206672	3.853734	0.000816
Sr	-1.477699	0.000319	0.002475

E. Ba@C_1(17459)-C_{76}.

Coordinates:

C	-0.013811	-0.059430	0.106072
C	1.373823	-0.049497	0.103970
C	2.108965	1.193227	0.098339
C	3.298661	0.984575	-0.682888
C	3.936726	2.052171	-1.364434
C	4.588131	1.749310	-2.601410
C	4.740804	2.736306	-3.637149
C	4.671811	2.052038	-4.903089
C	4.161731	2.698325	-6.080585
C	3.410008	1.871890	-6.983484
C	2.212143	2.393456	-7.623658
C	1.202759	1.359105	-7.620610
C	-0.152284	1.604921	-7.252022
C	-0.918362	0.503288	-6.648907
C	-2.021014	0.797595	-5.724263
C	-2.398226	-0.155379	-4.730445
C	-2.796784	0.243988	-3.407441
C	-2.347289	-0.778405	-2.472209
C	-1.894093	-0.417062	-1.210619
C	-0.732245	-1.063393	-0.641753
C	-0.725156	1.206833	-0.003742
C	-1.877928	0.988344	-0.822973
C	-2.365357	1.999193	-1.697687

C	-2.836172	1.608861	-3.035926
C	-2.706152	2.547890	-4.100254
C	-2.295375	2.154596	-5.410001
C	-1.550906	3.242962	-6.013597
C	-0.508477	3.004172	-6.947496
C	0.477944	4.031408	-7.060112
C	1.843640	3.727450	-7.448898
C	2.724362	4.609133	-6.750582
C	3.798522	4.088045	-5.966625
C	3.722930	4.725294	-4.658575
C	4.175514	4.051848	-3.483209
C	3.493817	4.348496	-2.259756
C	3.389091	3.359996	-1.199089
C	2.155341	3.544449	-0.500350
C	1.440757	2.447927	0.075074
C	-0.027842	2.450915	-0.005515
C	-0.671934	3.520222	-0.694230
C	-1.805116	3.296559	-1.524850
C	-1.724061	4.247056	-2.630819
C	-2.179559	3.873143	-3.879263
C	-1.463798	4.305175	-5.052758
C	-0.320634	5.158329	-4.962729
C	0.559412	5.113275	-6.083521
C	1.933828	5.474151	-5.935124
C	2.512470	5.535423	-4.637409
C	1.678009	5.594787	-3.470311
C	2.274708	5.109839	-2.261293
C	1.468835	4.624915	-1.165739
C	0.089633	4.620897	-1.279801
C	-0.540109	5.057236	-2.493420
C	0.221690	5.481285	-3.628723
C	2.100018	-1.007683	-0.710946
C	3.253762	-0.351740	-1.249727
C	3.668675	-0.580071	-2.589771
C	4.415293	0.464571	-3.214310
C	4.430471	0.653720	-4.634801
C	3.620311	-0.149483	-5.489514
C	3.172173	0.472731	-6.693188
C	1.864799	0.151562	-7.201698
C	1.139066	-0.885557	-6.665846
C	-0.279737	-0.758937	-6.495522
C	-0.654788	-1.696530	-5.457811
C	-1.718119	-1.428027	-4.616502
C	-1.665848	-1.810870	-3.218835

C	-0.510643	-2.402081	-2.697308
C	-0.029147	-2.021427	-1.392346
C	1.415521	-1.955468	-1.460220
C	1.832097	-2.219621	-2.827178
C	2.898682	-1.500112	-3.437528
C	2.839189	-1.251784	-4.888868
C	1.680783	-1.684395	-5.584283
C	0.562014	-2.279260	-4.910987
C	0.645136	-2.583362	-3.562172
Ba	1.527445	2.414659	-4.298835

F. Ba@*C*$_{2v}$(19138)-C$_{76}$.

Coordinates:

C	0.888726	-0.710007	-3.697291
C	-0.512644	-1.141484	-3.699007
C	1.900975	-1.463920	-3.033798
C	1.511498	-2.691904	-2.319809
C	0.135058	-3.092459	-2.358605
C	-0.860263	-2.311115	-3.054574
C	-1.914600	-3.249664	-1.226909
C	-2.118097	-2.382700	-2.346003
C	-0.515573	-3.656603	-1.224822
C	-0.510488	1.141691	-3.698593
C	-1.380946	0.000926	-3.671168
C	0.890061	0.707558	-3.697027
C	-3.025959	-1.266953	-2.306037
C	-2.614059	0.001961	-2.928415
C	-3.904535	-1.232239	-1.173485
C	-3.649674	-2.056842	-0.000268
C	-2.615689	-3.033909	-0.000342
C	-4.441677	0.003041	0.715540
C	-4.441667	0.003295	-0.715436
C	-3.904470	-1.232583	1.173115
C	-3.023600	1.271441	-2.305618
C	-3.902225	1.237977	-1.173055
C	0.140885	3.090965	-2.357495
C	-0.855904	2.311753	-3.053744
C	1.516562	2.687777	-2.318837
C	1.903722	1.459318	-3.033265
C	-2.113600	2.385461	-2.345150
C	-1.908497	3.251683	-1.225761

C	-0.508691	3.655942	-1.223515
C	-3.645834	2.061689	0.000465
C	-2.610003	3.036820	0.000739
C	3.023024	0.712756	-2.569359
C	3.021681	-0.719627	-2.569622
C	3.803943	1.154241	-1.419168
C	3.394551	2.285068	-0.723516
C	2.259487	3.061469	-1.172277
C	3.801765	-1.162986	-1.419581
C	4.273859	-0.004942	-0.705187
C	-3.902161	1.237487	1.173565
C	-3.023468	1.270513	2.306001
C	-2.613954	0.000916	2.928293
C	-3.025835	-1.267671	2.305522
C	-1.914705	-3.250210	1.226126
C	-2.118178	-2.383494	2.345404
C	-0.856118	2.310656	3.054975
C	-2.113684	2.384590	2.346256
C	-0.510752	1.140375	3.699408
C	-1.381165	-0.000382	3.671437
C	-1.908601	3.251356	1.227293
C	-0.860476	-2.312194	3.054156
C	0.134891	-3.093308	2.357991
C	-0.515659	-3.657106	1.223988
C	0.193110	-3.854464	-0.000424
C	-0.512907	-1.142805	3.699007
C	0.888455	-0.711327	3.697582
C	1.900740	-1.465000	3.033915
C	1.511310	-2.692739	2.319448
C	0.889789	0.706239	3.697821
C	-0.508779	3.655576	1.225291
C	0.140718	3.090136	2.359088
C	1.903487	1.458233	3.034429
C	1.516375	2.686960	2.320401
C	3.390177	-2.293547	0.724259
C	2.253643	-3.067850	1.172946
C	3.390236	-2.293280	-0.724334
C	2.253723	-3.067402	-1.173379
C	1.589442	-3.584905	-0.000327
C	3.801628	-1.163488	1.419926
C	3.021482	-0.720535	2.570092
C	3.022822	0.711831	2.570338
C	3.803802	1.153728	1.420338
C	4.273782	-0.005194	0.705974

C	3.394493	2.284818	0.725076
C	2.259410	3.061083	1.174035
C	1.596182	3.579805	0.000954
C	0.200363	3.852029	0.000951
Ba	-1.098820	0.000382	-0.004493

IV. The simulated IR spectra of C_{76}^{2-}-C_1(17459), C_{76}^{2-}-C_{2v}(19138), M@C_1(17459)-C_{76} and M@C_{2v}(19138)-C_{76} (M=Ca, Sr, and Ba).

IR spectra of six endohedral metallofullerenes have been calculated theoretically to assist further experimental characterization. In addition, the IR spectra of two di-anions, C_{76}^{2-}-C_1(17459) and C_{76}^{2-}-C_{2v}(19138), have also simulated to compare with endohedral metallofullerenes.

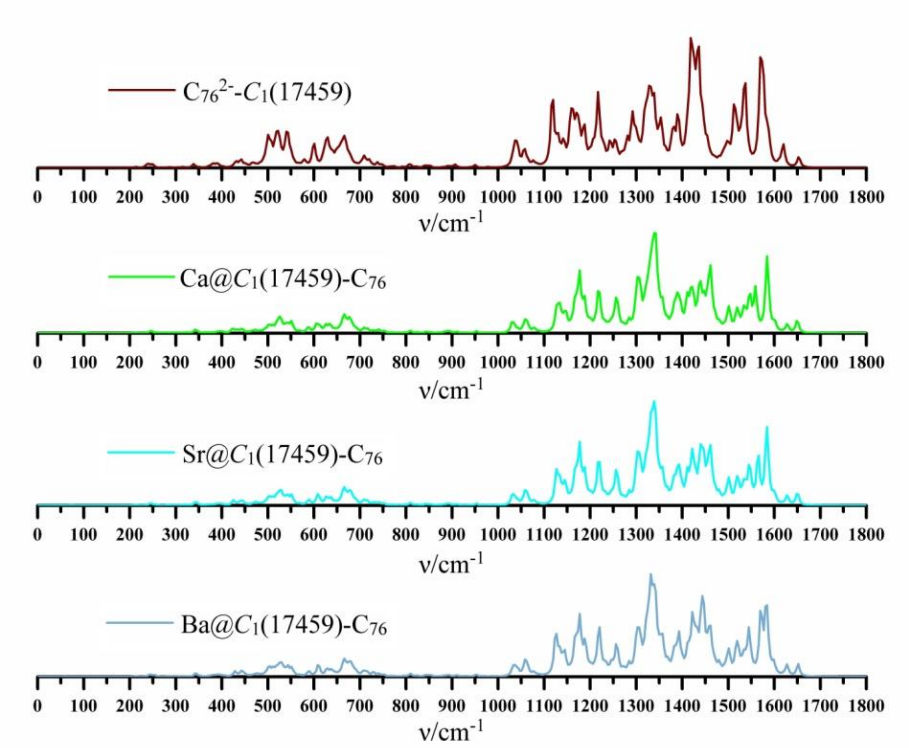

Fig. S1 Simulated IR spectra of C_{76}^{2-}-C_1(17459) and M@C_1(17459)-C_{76} (M=Ca, Sr, and Ba).

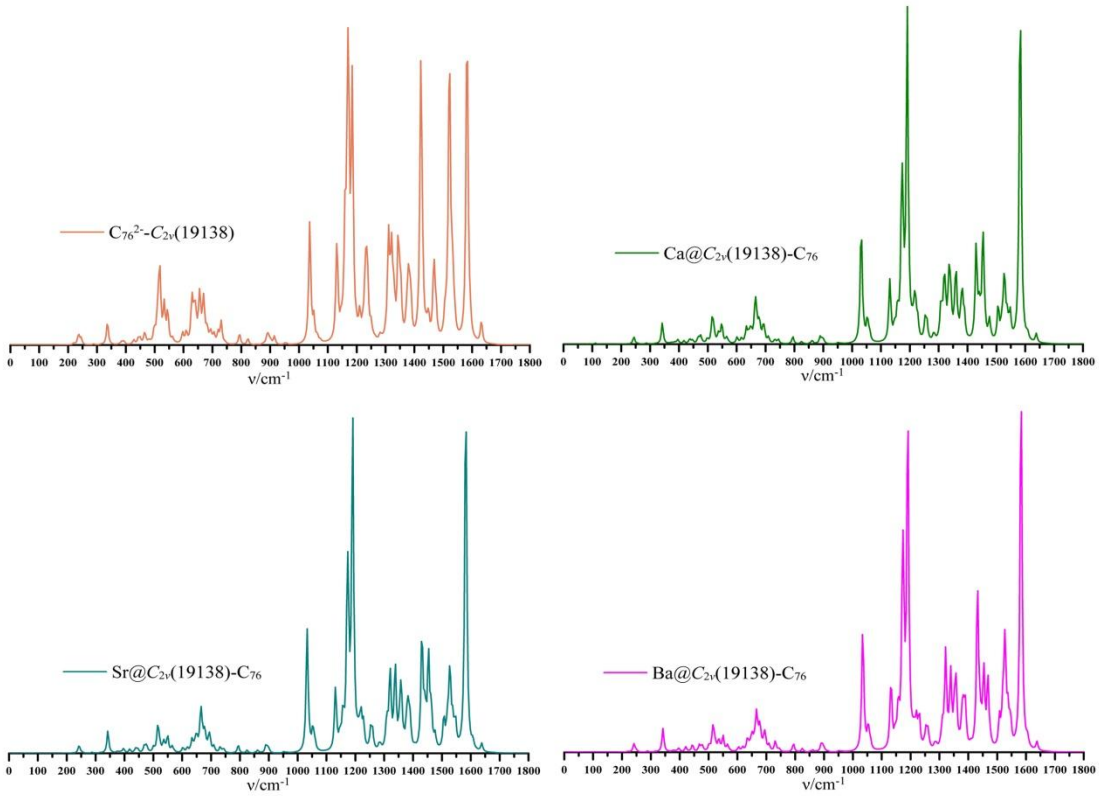

Fig. S2 Simulated IR spectra of C_{76}^{2-}-C_{2v}(19138) and M@C_{2v}(19138)-C_{76} (M=Ca, Sr, and Ba)