Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Ground and Excited Electronic Structures of Metal Encapsulated Nanocages: The Cases of Endohedral $M@C_{20}H_{20}$ (M = K, Rb, Ca, Sr) and $M@C_{36}H_{36}$ (M = Na, K, Rb)

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Supporting Information

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Table S1. Optimized geometries (Cartesian coordinates in Å) of M@$C_{20}H_{20}$ (M=K, K^+, Rb, Rb^+, Ca, Ca^+, Ca^{2+}, Sr, Sr^{2+}) at B3LYP/aug-cc-pVTZ Relativistic pseudopotentials that replace 28 core electrons, were combined with aug-cc-pVTZ-PP basis set for M = Rb, Sr atoms.

K@$C_{20}H_{20}$			K@$C_{20}H_{20}^+$			Rb@$C_{20}H_{20}$			Rb@$C_{20}H_{20}^+$		
C	1.307151	-0.424719	C	1.307751	-0.424914	C	1.328793	-0.431751	C	1.329788	-0.432074
C	-1.307151	0.424719	C	-1.307751	0.424914	C	-1.328793	0.431751	C	-1.329788	0.432074
C	-0.000000	-1.374419	C	-0.000000	-1.375051	C	-0.000000	-1.397176	C	-0.000000	-1.398222
C	0.807863	1.111929	C	0.808235	1.112440	C	0.821239	1.130339	C	0.821854	1.131185
C	2.115014	-0.687210	C	2.115986	-0.687525	C	2.150032	-0.698588	C	2.151642	-0.699111
C	-0.807863	-1.111929	C	-0.808235	-1.112440	C	-0.821239	-1.130339	C	-0.821854	-1.131185
C	0.000000	1.374419	C	0.000000	1.375051	C	-0.000000	1.397176	C	0.000000	1.398222
C	-2.115014	0.687210	C	-2.115986	0.687525	C	-2.150032	0.698588	C	-2.151642	0.699111
C	-0.000000	-2.223857	C	-0.000000	-2.224879	C	0.000000	-2.260678	C	-0.000000	-2.262370
C	-1.307151	-0.424719	C	-1.307751	-0.424914	C	-1.328793	-0.431751	C	-1.329788	-0.432074
C	-0.807863	1.111929	C	-0.808235	1.112440	C	-0.821239	1.130339	C	-0.821854	1.131185
C	1.307151	1.799138	C	1.307751	1.799965	C	1.328793	1.828927	C	1.329788	1.830296
C	2.115014	0.687210	C	2.115986	0.687525	C	2.150032	0.698588	C	2.151642	0.699111
C	1.307151	-1.799138	C	1.307751	-1.799965	C	1.328793	-1.828927	C	1.329788	-1.830296
C	-1.307151	-1.799138	C	-1.307751	-1.799965	C	-1.328793	-1.828927	C	-1.329788	-1.830296
C	0.807863	-1.111929	C	0.808235	-1.112440	C	0.821239	-1.130339	C	0.821854	-1.131185
C	1.307151	0.424719	C	1.307751	0.424914	C	1.328793	0.431751	C	1.329788	0.432074
C	0.000000	2.223857	C	-0.000000	2.224879	C	-0.000000	2.260678	C	0.000000	2.262370
C	-1.307151	1.799138	C	-1.307751	1.799965	C	-1.328793	1.828927	C	-1.329788	1.830296
C	-2.115014	-0.687210	C	-2.115986	-0.687525	C	-2.150032	-0.698588	C	-2.151642	-0.699111
H	1.934115	-0.628432	H	1.933339	-0.628180	H	1.956241	-0.635621	H	1.955967	-0.635532
H	-1.934115	0.628432	H	-1.933339	0.628180	H	-1.956241	0.635621	H	-1.955967	0.635532
H	-0.000000	-2.033649	H	-0.000000	-2.032833	H	-0.000000	-2.056914	H	-0.000000	-2.056626
H	1.195349	1.645257	H	1.194869	1.644596	H	1.209023	1.664078	H	1.208854	1.663845
H	3.129465	-1.016825	H	3.128208	-1.016417	H	3.165265	-1.028457	H	3.164821	-1.028313
H	-1.195349	-1.645257	H	-1.194869	-1.644596	H	-1.209023	-1.664078	H	-1.208854	-1.663845
H	0.000000	2.033649	H	0.000000	2.032833	H	0.000000	2.056914	H	0.000000	2.056626
H	-3.129465	1.016825	H	-3.128208	1.016417	H	-3.165265	1.028457	H	-3.164821	1.028313
H	-0.000000	-3.290514	H	-0.000000	-3.289193	H	0.000000	-3.328156	H	-0.000000	-3.327690
H	-1.934115	-0.628432	H	-1.933339	-0.628180	H	-1.956241	-0.635621	H	-1.955967	-0.635532
H	-1.195349	1.645257	H	-1.194869	1.644596	H	-1.209023	1.664078	H	-1.208854	1.663845
H	1.934115	2.662082	H	1.933339	2.661013	H	1.956241	2.692535	H	1.955967	2.692158
H	3.129465	1.016825	H	3.128208	1.016417	H	3.165265	1.028457	H	3.164821	1.028313
H	1.934115	-2.662082	H	1.933339	-2.661013	H	1.956241	-2.692535	H	1.955967	-2.692158
H	-1.934115	-2.662082	H	-1.933339	-2.661013	H	-1.956241	-2.692535	H	-1.955967	-2.692158
H	1.195349	-1.645257	H	1.194869	-1.644596	H	1.209023	-1.664078	H	1.208854	-1.663845
H	1.934115	0.628432	H	1.933339	0.628180	H	1.956241	0.635621	H	1.955967	0.635532
H	0.000000	3.290514	H	-0.000000	3.289193	H	-0.000000	3.328156	H	0.000000	3.327690
H	-1.934115	2.662082	H	-1.933339	2.661013	H	-1.956241	2.692535	H	-1.955967	2.692158
H	-3.129465	-1.016825	H	-3.128208	-1.016417	H	-3.165265	-1.028457	H	-3.164821	-1.028313
K	0.000000	0.000000	K	0.000000	0.000000	Rb	0.000000	0.000000	Rb	0.000000	0.000000

Ca@$C_{20}H_{20}$			Ca@$C_{20}H_{20}^+$			Ca@$C_{20}H_{20}^{2+}$			Sr@$C_{20}H_{20}$		
C	1.299669	-0.422288	C	0.000000	-1.367630	C	1.302899	-0.423338	C	1.323656	-0.430082
C	-1.299669	0.422288	C	0.000000	1.367630	C	-1.302899	0.423338	C	-1.323656	0.430082
C	-0.000000	-1.366553	C	-1.300694	-0.422621	C	-0.000000	-1.369949	C	-0.000000	-1.391774
C	0.803240	1.105565	C	1.300694	-0.422621	C	0.805236	1.108312	C	0.818064	1.125969
C	2.102909	-0.683276	C	0.000000	-2.212873	C	2.108135	-0.684975	C	2.141720	-0.695887
C	-0.803240	-1.105565	C	-1.300694	0.422621	C	-0.805236	-1.108312	C	-0.818064	-1.125969
C	0.000000	1.366553	C	1.300694	0.422621	C	0.000000	1.369949	C	0.000000	1.391774
C	-2.102909	0.683276	C	0.000000	2.212873	C	-2.108135	0.684975	C	-2.141720	0.695887
C	-0.000000	-2.211129	C	-2.104567	-0.683815	C	0.000000	-2.216625	C	-0.000000	-2.251937
C	-1.299669	-0.422288	C	-0.803873	1.106436	C	-1.302899	-0.423338	C	-1.323656	-0.430082
C	-0.803240	1.105565	C	0.803873	1.106436	C	-0.805236	1.108312	C	-0.818064	1.125969
C	1.299669	1.788841	C	2.104567	-0.683815	C	1.302899	1.793287	C	1.323656	1.821856
C	2.102909	0.683276	C	1.300694	-1.790251	C	2.108135	0.684975	C	2.141720	0.695887
C	1.299669	-1.788841	C	-1.300694	-1.790251	C	1.302899	-1.793287	C	1.323656	-1.821856
C	-1.299669	-1.788841	C	-2.104567	0.683815	C	-1.302899	-1.793287	C	-1.323656	-1.821856
C	0.803240	-1.105565	C	-0.803873	-1.106436	C	0.805236	-1.108312	C	0.818064	-1.125969
C	1.299669	0.422288	C	0.803873	-1.106436	C	1.302899	0.423338	C	1.323656	0.430082
C	0.000000	2.211129	C	2.104567	0.683815	C	-0.000000	2.216625	C	0.000000	2.251937
C	-1.299669	1.788841	C	1.300694	1.790251	C	-1.302899	1.793287	C	-1.323656	1.821856
C	-2.102909	-0.683276	C	-1.300694	1.790251	C	-2.108135	-0.684975	C	-2.141720	-0.695887
H	1.928421	-0.626582	H	0.000000	-2.027276	H	1.927365	-0.626239	H	1.951526	-0.634089
H	-1.928421	0.626582	H	0.000000	2.027276	H	-1.927365	0.626239	H	-1.951526	0.634089
H	-0.000000	-2.027661	H	-1.928054	-0.626463	H	-0.000000	-2.026552	H	-0.000000	-2.051956
H	1.191829	1.640412	H	1.928054	-0.626463	H	1.191177	1.639515	H	1.206109	1.660067
H	3.120250	-1.013831	H	0.000000	-3.280202	H	3.118543	-1.013276	H	3.157636	-1.025978
H	-1.191829	-1.640412	H	-1.928054	0.626463	H	-1.191177	-1.639515	H	-1.206109	-1.660067
H	0.000000	2.027661	H	1.928054	0.626463	H	0.000000	2.026552	H	0.000000	2.051956
H	-3.120250	1.013831	H	0.000000	3.280202	H	-3.118543	1.013276	H	-3.157636	1.025978
H	-0.000000	-3.280825	H	-3.119657	-1.013638	H	-0.000000	-3.279030	H	-0.000000	-3.320135
H	-1.928421	-0.626582	H	-1.191603	1.640101	H	-1.927365	-0.626239	H	-1.951526	-0.634089
H	-1.191829	1.640412	H	1.191603	1.640101	H	-1.191177	1.639515	H	-1.206109	1.660067
H	1.928421	2.654243	H	3.119657	-1.013638	H	1.927365	2.652791	H	1.951526	2.686045
H	3.120250	1.013831	H	1.928054	-2.653739	H	3.118543	1.013276	H	3.157636	1.025978
H	1.928421	-2.654243	H	-1.928054	-2.653739	H	1.927365	-2.652791	H	1.951526	-2.686045
H	-1.928421	-2.654243	H	-3.119657	1.013638	H	-1.927365	-2.652791	H	-1.951526	-2.686045
H	1.191829	-1.640412	H	-1.191603	-1.640101	H	1.191177	-1.639515	H	1.206109	-1.660067
H	1.928421	0.626582	H	1.191603	-1.640101	H	1.927365	0.626239	H	1.951526	0.634089
H	0.000000	3.280825	H	3.119657	1.013638	H	0.000000	3.279030	H	0.000000	3.320135
H	-1.928421	2.654243	H	1.928054	2.653739	H	-1.927365	2.652791	H	-1.951526	2.686045
H	-3.120250	-1.013831	H	-1.928054	2.653739	H	-3.118543	-1.013276	H	-3.157636	-1.025978
Ca	0.000000	0.000000	Ca	0.000000	0.000000	Ca	0.000000	0.000000	Sr	0.000000	0.000000

Sr@$C_{20}H_{20}^{2+}$		
C	1.327443	-0.431312
C	-1.327443	0.431312
C	-0.000000	-1.395756
C	0.820405	1.129190
C	2.147847	-0.697878
C	-0.820405	-1.129190
C	0.000000	1.395756
C	-2.147847	0.697878
C	-0.000000	-2.258380
C	-1.327443	-0.431312
C	-0.820405	1.129190
C	1.327443	1.827068
C	2.147847	0.697878
C	1.327443	-1.827068

C	-1.327443	-1.827068	-0.431312
C	0.820405	-1.129190	-1.827068
C	1.327443	0.431312	-1.827068
C	0.000000	2.258380	-0.431312
C	-1.327443	1.827068	0.431312
C	-2.147847	-0.697878	0.431312
H	1.951776	-0.634170	2.686389
H	-1.951776	0.634170	-2.686389
H	-0.000000	-2.052219	2.686389
H	1.206264	1.660280	2.686389
H	3.158040	-1.026109	0.634170
H	-1.206264	-1.660280	-2.686389
H	0.000000	2.052219	-2.686389
H	-3.158040	1.026109	-0.634170
H	-0.000000	-3.320560	0.634170
H	-1.951776	-0.634170	2.686389
H	-1.206264	1.660280	2.686389
H	1.951776	2.686389	0.634170
H	3.158040	1.026109	-0.634170
H	1.951776	-2.686389	-0.634170
H	-1.951776	-2.686389	-0.634170
H	1.206264	-1.660280	-2.686389
H	1.951776	0.634170	-2.686389
H	0.000000	3.320560	-0.634170
H	-1.951776	2.686389	0.634170
H	-3.158040	-1.026109	0.634170
Sr	0.000000	0.000000	0.000000

Table S2. Optimized geometries (Cartesian coordinates in Å) of M@$C_{36}H_{36}$ (M=Na, Na^+, K, K^+, Rb, Rb^+) at B3LYP/aug-cc-pVDZ Relativistic pseudopotentials that replace 28 core electrons, were combined with aug-cc-pVDZ-PP basis set for M = Rb atom.

Na@$C_{36}H_{36}$				Na@$C_{36}H_{36}^+$				K@$C_{36}H_{36}$				K@$C_{36}H_{36}^+$			
C	-0.696687	2.603557	0.315130	C	-0.699411	2.609624	0.312254	C	-0.692171	2.605048	0.327456	C	-0.692937	2.608219	0.327588
C	0.696687	2.603557	-0.315130	C	0.699411	2.609624	-0.312254	C	0.692171	2.605048	-0.327456	C	0.692937	2.608219	-0.327588
C	1.616350	1.267596	1.854628	C	1.621391	1.268679	1.855043	C	1.618481	1.274330	1.881464	C	1.620447	1.275385	1.883066
C	0.145626	0.788452	2.214460	C	0.146342	0.790988	2.210579	C	0.147715	0.800702	2.302298	C	0.148004	0.801434	2.304283
C	1.830974	2.292222	0.674929	C	1.837803	2.297623	0.676215	C	1.820714	2.288197	0.671353	C	1.823716	2.291664	0.671605
C	-0.931630	1.796026	1.650757	C	-0.936192	1.799233	1.649144	C	-0.934425	1.807918	1.693700	C	-0.935945	1.809667	1.695769
C	-1.616350	-1.267596	1.854628	C	-1.621391	-1.268679	1.855043	C	-1.618481	-1.274330	1.881464	C	-1.620447	-1.275385	1.883066
C	-0.145626	-0.788452	2.214460	C	-0.146342	-0.790988	2.210579	C	-0.147715	-0.800702	2.302298	C	-0.148004	-0.801434	2.304283
C	0.931630	-1.796026	1.650757	C	0.936192	-1.799233	1.649144	C	0.934425	-1.807918	1.693700	C	0.935945	-1.809667	1.695769
C	-1.830974	-2.292222	0.674929	C	-1.837803	-2.297623	0.676215	C	-1.820714	-2.288197	0.671353	C	-1.823716	-2.291664	0.671605
C	-0.696687	-2.603557	-0.315130	C	-0.699411	-2.609624	-0.312254	C	-0.692171	-2.605048	-0.327456	C	-0.692937	-2.608219	-0.327588
C	0.696687	-2.603557	0.315130	C	0.699411	-2.609624	0.312254	C	0.692171	-2.605048	0.327456	C	0.692937	-2.608219	0.327588
C	-2.415013	1.316821	1.574761	C	-2.421217	1.319773	1.574623	C	-2.415320	1.317924	1.586354	C	-2.418643	1.319429	1.587476
C	-2.752966	-0.194632	1.726681	C	-2.759300	-0.193698	1.726745	C	-2.751768	-0.196334	1.735557	C	-2.755489	-0.196479	1.736704
C	2.998320	1.794966	-0.200611	C	3.005995	1.798167	-0.199646	C	2.987560	1.791550	-0.202453	C	2.992239	1.793988	-0.202331
C	2.752966	0.194632	1.726681	C	2.759300	0.193698	1.726745	C	2.751768	0.196334	1.735557	C	2.755489	0.196479	1.736704
C	2.415013	-1.316821	1.574761	C	2.421217	-1.319773	1.574623	C	2.415320	-1.317924	1.586354	C	2.418643	-1.319429	1.587476
C	3.645508	0.588507	0.501740	C	3.652374	0.588937	0.502004	C	3.635738	0.588412	0.501559	C	3.640502	0.589050	0.501880
C	3.645508	-0.588507	-0.501740	C	3.652374	-0.588937	-0.502004	C	3.635738	-0.588412	-0.501559	C	3.640502	-0.589050	-0.501880
C	2.998320	-1.794966	0.200611	C	3.005995	-1.798167	0.199646	C	2.987560	-1.791550	0.202453	C	2.992239	-1.793988	0.202331
C	2.752966	-0.194632	-1.726681	C	2.759300	-0.193698	-1.726745	C	2.751768	-0.196334	-1.735557	C	2.755489	-0.196479	-1.736704
C	2.415013	1.316821	-1.574761	C	2.421217	1.319773	-1.574623	C	2.415320	1.317924	-1.586354	C	2.418643	1.319429	-1.587476
C	0.931630	1.796026	-1.650757	C	0.936192	1.799233	-1.649144	C	0.934425	1.807918	-1.693700	C	0.935945	1.809667	-1.695769
C	-0.145626	0.788452	-2.214460	C	-0.146342	0.790988	-2.210579	C	-0.147715	0.800702	-2.302298	C	-0.148004	0.801434	-2.304283
C	-1.616350	1.267596	-1.854628	C	-1.621391	1.268679	-1.855043	C	-1.618481	1.274330	-1.881464	C	-1.620447	1.275385	-1.883066
C	-1.830974	2.292222	-0.674929	C	-1.837803	2.297623	-0.676215	C	-1.820714	2.288197	-0.671353	C	-1.823716	2.291664	-0.671605
C	1.830974	-2.292222	-0.674929	C	1.837803	-2.297623	-0.676215	C	1.820714	-2.288197	-0.671353	C	1.823716	-2.291664	-0.671605
C	1.616350	-1.267596	-1.854628	C	1.621391	-1.268679	-1.855043	C	1.618481	-1.274330	-1.881464	C	1.620447	-1.275385	-1.883066
C	0.145626	-0.788452	-2.214460	C	0.146342	-0.790988	-2.210579	C	0.147715	-0.800702	-2.302298	C	0.148004	-0.801434	-2.304283
C	-2.998320	1.794966	0.200611	C	-3.005995	1.798167	0.199646	C	-2.987560	1.791550	0.202453	C	-2.992239	1.793988	0.202331
C	-3.645508	0.588507	-0.501740	C	-3.652374	0.588937	-0.502004	C	-3.635738	0.588412	-0.501559	C	-3.640502	0.589050	-0.501880
C	-0.931630	-1.796026	-1.650757	C	-0.936192	-1.799233	-1.649144	C	-0.934425	-1.807918	-1.693700	C	-0.935945	-1.809667	-1.695769
C	-2.415013	-1.316821	-1.574761	C	-2.421217	-1.319773	-1.574623	C	-2.415320	-1.317924	-1.586354	C	-2.418643	-1.319429	-1.587476
C	-2.752966	0.194632	-1.726681	C	-2.759300	0.193698	-1.726745	C	-2.751768	0.196334	-1.735557	C	-2.755489	0.196479	-1.736704
C	-2.998320	-1.794966	-0.200611	C	-3.005995	-1.798167	-0.199646	C	-2.987560	-1.791550	-0.202453	C	-2.992239	-1.793988	-0.202331
C	-3.645508	-0.588507	0.501740	C	-3.652374	-0.588937	0.502004	C	-3.635738	-0.588412	0.501559	C	-3.640502	-0.589050	0.501880
H	0.876249	3.643498	-0.627985	H	0.880498	3.644008	-0.625839	H	0.871322	3.645043	-0.634197	H	0.873422	3.643905	-0.635165
H	-0.876249	3.643498	0.627985	H	-0.880498	3.644008	0.625839	H	-0.871322	3.645043	0.634197	H	-0.873422	3.643905	0.635165
H	-2.102703	3.243426	-1.155469	H	-2.111067	3.243554	-1.157364	H	-2.089146	3.242893	-1.145611	H	-2.093106	3.242665	-1.144168
H	-3.722291	2.603629	0.368106	H	-3.730760	2.602717	0.367104	H	-3.710549	2.602379	0.365376	H	-3.715215	2.601080	0.365109
H	-4.664467	0.819351	-0.839398	H	-4.669361	0.818224	-0.838906	H	-4.655965	0.821718	-0.834429	H	-4.658623	0.821030	-0.833256
H	-3.357894	0.286234	-2.639086	H	-3.362568	0.284567	-2.635919	H	-3.365699	0.285790	-2.642169	H	-3.368627	0.285285	-2.639373
H	-1.888246	1.851397	-2.744504	H	-1.892819	1.848440	-2.741204	H	-1.915710	1.872538	-2.751756	H	-1.918900	1.871199	-2.749327
H	-0.079768	0.989584	-3.289488	H	-0.077869	0.987613	-3.279739	H	-0.096460	1.020331	-3.372134	H	-0.096457	1.019226	-3.371716
H	0.903402	2.578853	-2.421836	H	0.905443	2.578495	-2.415780	H	0.923528	2.603269	-2.449055	H	0.926270	2.602455	-2.448464
H	2.102703	3.243426	1.155469	H	2.111067	3.243554	1.157364	H	2.089146	3.242893	1.145611	H	2.093106	3.242665	1.144168
H	3.722291	2.603629	-0.368106	H	3.730760	2.602717	-0.367104	H	3.710549	2.602379	-0.365376	H	3.715215	2.601080	-0.365109
H	2.957606	1.838226	-2.375107	H	2.963134	1.838830	-2.372037	H	2.974712	1.835353	-2.377856	H	2.978012	1.834718	-2.375137
H	4.664467	0.819351	0.839398	H	4.669361	0.818224	0.838906	H	4.655965	0.821718	0.834429	H	4.658623	0.821030	0.833256
H	4.664467	-0.819351	-0.839398	H	4.669361	-0.818224	-0.838906	H	4.655965	-0.821718	-0.834429	H	4.658623	-0.821030	-0.833256
H	3.357894	-0.286234	-2.639086	H	3.362568	-0.284567	-2.635919	H	3.365699	-0.285790	-2.642169	H	3.368627	-0.285285	-2.639373
H	1.888246	-1.851397	-2.744504	H	1.892819	-1.848440	-2.741204	H	1.915710	-1.872538	-2.751756	H	1.918900	-1.871199	-2.749327
H	0.079768	-0.989584	-3.289488	H	0.077869	-0.987613	-3.279739	H	0.096460	-1.020331	-3.372134	H	0.096457	-1.019226	-3.371716
H	-0.903402	-2.578853	-2.421836	H	-0.905443	-2.578495	-2.415780	H	-0.923528	-2.603269	-2.449055	H	-0.926270	-2.602455	-2.448464
H	-2.957606	-1.838226	-2.375107	H	-2.963134	-1.838830	-2.372037	H	-2.974712	-1.835353	-2.377856	H	-2.978012	-1.834718	-2.375137
H	-4.664467	-0.819351	0.839398	H	-4.669361	-0.818224	0.838906	H	-4.655965	-0.821718	0.834429	H	-4.658623	-0.821030	0.833256
H	-3.722291	-2.603629	-0.368106	H	-3.730760	-2.602717	-0.367104	H	-3.710549	-2.602379	-0.365376	H	-3.715215	-2.601080	-0.365109
H	-2.102703	-3.243426	1.155469	H	-2.111067	-3.243554	1.157364	H	-2.089146	-3.242893	1.145611	H	-2.093106	-3.242665	1.144168
H	-0.876249	-3.643498	-0.627985	H	-0.880498	-3.644008	-0.625839	H	-0.871322	-3.645043	-0.634197	H	-0.873422	-3.643905	-0.635165
H	0.876249	-3.643498	0.627985	H	0.880498	-3.644008	0.625839	H	0.871322	-3.645043	0.634197	H	0.873422	-3.643905	0.635165
H	0.903402	-2.578853	2.421836	H	0.905443	-2.578495	2.415780	H	0.923528	-2.603269	2.449055	H	0.926270	-2.602455	2.448464
H	2.102703	-3.243426	-1.155469	H	2.111067	-3.243554	-1.157364	H	2.089146	-3.242893	-1.145611	H	2.093106	-3.242665	-1.144168
H	3.722291	-2.603629	0.368106	H	3.730760	-2.602717	0.367104	H	3.710549	-2.602379	0.365376	H	3.715215	-2.601080	0.365109
H	2.957606	-1.838226	2.375107	H	2.963134	-1.838830	2.372037	H	2.974712	-1.835353	2.377856	H	2.978012	-1.834718	2.375137
H	3.357894	0.286234	2.639086	H	3.362568	0.284567	2.635919	H	3.365699	0.285790	2.642169	H	3.368627	0.285285	2.639373
H	0.079768	0.989584	3.289488	H	0.077869	0.987613	3.279739	H	0.096460	1.020331	3.372134	H	0.096457	1.019226	3.371716
H	1.888246	1.851397	2.744504	H	1.892819	1.848440	2.741204	H	1.915710	1.872538	2.751756	H	1.918900	1.871199	2.749327
H	-0.079768	-0.989584	3.289488	H	-0.077869	-0.987613	3.279739	H	-0.096460	-1.020331	3.372134	H	-0.096457	-1.019226	3.371716
H	-1.888246	-1.851397	2.744504	H	-1.892819	-1.848440	2.741204	H	-1.915710	-1.872538	2.751756	H	-1.918900	-1.871199	2.749327
H	-3.357894	-0.286234	2.639086	H	-3.362568	-0.284567	2.635919	H	-3.365699	-0.285790	2.642169	H	-3.368627	-0.285285	2.639373

H	-2.957606	1.838226	2.375107	H	-2.963134	1.838830	2.372037	H	-2.974712	1.835353	2.377856	H	-2.978012	1.834718	2.375137
H	-0.903402	2.578853	2.421836	H	-0.905443	2.578495	2.415780	H	-0.923528	2.603269	2.449055	H	-0.926270	2.602455	2.448464
Na	0.000000	0.000000	0.000000	Na	0.000000	0.000000	0.000000	K	0.000000	0.000000	0.000000	K	0.000000	0.000000	0.000000
	$Rb@C_{36}H_{36}$				$Rb@C_{36}H_{36}^{+}$													
C	-0.690757	2.619444	0.334196	C	-0.691340	2.622241	0.334375											
C	0.690757	2.619444	-0.334196	C	0.691340	2.622241	-0.334375											
C	1.619081	1.282872	1.899167	C	1.620492	1.283708	1.900461											
C	0.148985	0.810943	2.348756	C	0.149216	0.811501	2.350563											
C	1.815899	2.292680	0.670845	C	1.818494	2.295914	0.671058											
C	-0.935810	1.822855	1.718837	C	-0.936893	1.824277	1.720737											
C	-1.619081	-1.282872	1.899167	C	-1.620492	-1.283708	1.900461											
C	-0.148985	-0.810943	2.348756	C	-0.149216	-0.811501	2.350563											
C	0.935810	-1.822855	1.718837	C	0.936893	-1.824277	1.720737											
C	-1.815899	-2.292680	0.670845	C	-1.818494	-2.295914	0.671058											
C	-0.690757	-2.619444	-0.334196	C	-0.691340	-2.622241	-0.334375											
C	0.690757	-2.619444	0.334196	C	0.691340	-2.622241	0.334375											
C	-2.412886	1.320277	1.592843	C	-2.415615	1.321578	1.593862											
C	-2.747402	-0.197813	1.741251	C	-2.750673	-0.198089	1.742346											
C	2.979856	1.790559	-0.203267	C	2.984222	1.792962	-0.203243											
C	2.747402	0.197813	1.741251	C	2.750673	0.198089	1.742346											
C	2.412886	-1.320277	1.592843	C	2.415615	-1.321578	1.593862											
C	3.626580	0.588150	0.501758	C	3.631294	0.588880	0.502109											
C	3.626580	-0.588150	-0.501758	C	3.631294	-0.588880	-0.502109											
C	2.979856	-1.790559	0.203267	C	2.984222	-1.792962	0.203243											
C	2.747402	-0.197813	-1.741251	C	2.750673	-0.198089	-1.742346											
C	2.412886	1.320277	-1.592843	C	2.415615	1.321578	-1.593862											
C	0.935810	1.822855	-1.718837	C	0.936893	1.824277	-1.720737											
C	-0.148985	0.810943	-2.348756	C	-0.149216	0.811501	-2.350563											
C	-1.619081	1.282872	-1.899167	C	-1.620492	1.283708	-1.900461											
C	-1.815899	2.292680	-0.670845	C	-1.818494	2.295914	-0.671058											
C	1.815899	-2.292680	-0.670845	C	1.818494	-2.295914	-0.671058											
C	1.619081	-1.282872	-1.899167	C	1.620492	-1.283708	-1.900461											
C	0.148985	-0.810943	-2.348756	C	0.149216	-0.811501	-2.350563											
C	-2.979856	1.790559	0.203267	C	-2.984222	1.792962	0.203243											
C	-3.626580	0.588150	-0.501758	C	-3.631294	0.588880	-0.502109											
C	-0.935810	-1.822855	-1.718837	C	-0.936893	-1.824277	-1.720737											
C	-2.412886	-1.320277	-1.592843	C	-2.415615	-1.321578	-1.593862											
C	-2.747402	0.197813	-1.741251	C	-2.750673	0.198089	-1.742346											
C	-2.979856	-1.790559	-0.203267	C	-2.984222	-1.792962	-0.203243											
C	-3.626580	-0.588150	0.501758	C	-3.631294	-0.588880	0.502109											
H	0.873466	3.659226	-0.637977	H	0.875185	3.658197	-0.638831											
H	-0.873466	3.659226	0.637977	H	-0.875185	3.658197	0.638831											
H	-2.088392	3.247788	-1.141348	H	-2.091840	3.247413	-1.139965											
H	-3.704621	2.600279	0.364744	H	-3.708476	2.599322	0.364103											
H	-4.647762	0.821639	-0.831870	H	-4.650245	0.821031	-0.830758											
H	-3.367868	0.284497	-2.643633	H	-3.369981	0.284210	-2.640984											
H	-1.932051	1.887256	-2.759322	H	-1.934104	1.885726	-2.757186											
H	-0.103425	1.037074	-3.417877	H	-0.103564	1.036164	-3.417931											
H	0.936540	2.623034	-2.468635	H	0.938732	2.622001	-2.468556											
H	2.088392	3.247788	1.141348	H	2.091840	3.247413	1.139965											
H	3.704621	2.600279	-0.364744	H	3.708476	2.599322	-0.364103											
H	2.984428	1.833592	-2.378345	H	2.986604	1.832848	-2.375740											
H	4.647762	0.821639	0.831870	H	4.650245	0.821031	0.830758											
H	4.647762	-0.821639	-0.831870	H	4.650245	-0.821031	-0.830758											
H	3.367868	-0.284497	-2.643633	H	3.369981	-0.284210	-2.640984											
H	1.932051	-1.887256	-2.759322	H	1.934104	-1.885726	-2.757186											
H	0.103425	-1.037074	-3.417877	H	0.103564	-1.036164	-3.417931											
H	-0.936540	-2.623034	-2.468635	H	-0.938732	-2.622001	-2.468556											
H	-2.984428	-1.833592	-2.378345	H	-2.986604	-1.832848	-2.375740											
H	-4.647762	-0.821639	0.831870	H	-4.650245	-0.821031	0.830758											
H	-3.704621	-2.600279	-0.364744	H	-3.708476	-2.599322	-0.364103											
H	-2.088392	-3.247788	1.141348	H	-2.091840	-3.247413	1.139965											
H	-0.873466	-3.659226	-0.637977	H	-0.875185	-3.658197	-0.638831											
H	0.873466	-3.659226	0.637977	H	0.875185	-3.658197	0.638831											
H	0.936540	-2.623034	2.468635	H	0.938732	-2.622001	2.468556											
H	2.088392	-3.247788	-1.141348	H	2.091840	-3.247413	-1.139965											
H	3.704621	-2.600279	0.364744	H	3.708476	-2.599322	0.364103											
H	2.984428	-1.833592	2.378345	H	2.986604	-1.832848	2.375740											
H	3.367868	0.284497	2.643633	H	3.369981	0.284210	2.640984											
H	0.103425	1.037074	3.417877	H	0.103564	1.036164	3.417931											
H	1.932051	1.887256	2.759322	H	1.934104	1.885726	2.757186											
H	-0.103425	-1.037074	3.417877	H	-0.103564	-1.036164	3.417931											
H	-1.932051	-1.887256	2.759322	H	-1.934104	-1.885726	2.757186											
H	-3.367868	-0.284497	2.643633	H	-3.369981	-0.284210	2.640984											
H	-2.984428	1.833592	2.378345	H	-2.986604	1.832848	2.375740											
H	-0.936540	2.623034	2.468635	H	-0.938732	2.622001	2.468556											
Rb	0.000000	0.000000	0.000000	Rb	0.000000	0.000000	0.000000											

Table S3. DFT/B3LYP harmonic vibrational frequencies (cm^{-1}).

Harmonic vibrational frequencies (cm^{-1}) of $M@C_{20}H_{20}$									Harmonic vibrational frequencies (cm^{-1}) of $M@C_{36}H_{36}$					
M=K	$M=K^+$	M=Rb	$M=Rb^+$	M=Ca	$M=Ca^+$	$M=Ca^{2+}$	M=Sr	$M=Sr^{2+}$	M=Na	$M=Na^+$	M=K	$M=K^+$	M=Rb	$M=Rb^+$
436.1	438.8	345.1	346.5	402.2	399.7	409.0	329.7	334.8	50.4	28.5	82.4	80.0	78.0	76.6
436.8	438.8	345.6	346.5	403.1	400.6	409.8	330.3	335.3	188.7	184.8	230.8	229.7	210.3	209.4
436.8	438.8	345.6	346.5	403.3	400.8	410.1	330.3	335.4	224.5	221.5	244.5	243.4	233.3	232.4
484.4	484.3	465.9	465.6	487.6	486.5	484.0	467.7	463.8	244.3	242.4	248.2	247.7	233.6	233.1
484.5	484.3	466.0	465.6	487.7	486.6	484.1	467.8	463.9	281.5	278.9	296.5	295.4	283.6	282.6
484.8	484.3	466.3	465.6	488.0	486.9	484.5	468.1	464.2	289.9	287.7	303.5	303.0	301.2	300.1
485.0	484.3	466.6	465.6	488.3	487.2	484.7	468.4	464.5	292.9	292.1	304.9	304.0	303.2	302.8
485.2	484.3	466.7	465.6	488.4	487.3	484.8	468.5	464.5	295.5	293.6	316.3	315.4	308.6	307.7
559.9	560.1	555.1	555.6	543.7	542.2	543.1	547.5	546.2	312.4	310.3	322.9	322.0	325.5	324.8
560.0	560.1	555.2	555.6	543.8	542.3	543.2	547.6	546.4	314.0	313.9	331.6	329.8	332.9	332.0
560.1	560.1	555.4	555.6	543.9	542.4	543.3	547.8	546.6	327.6	325.8	346.7	345.7	357.8	356.8
560.2	560.1	555.4	555.6	544.0	542.5	543.4	547.8	546.6	380.2	378.3	384.1	382.9	388.3	387.1
560.2	560.1	555.6	555.6	544.1	542.6	543.5	548.0	546.8	414.8	412.0	423.2	422.0	426.6	425.6
619.4	619.3	609.0	608.7	625.1	624.5	623.3	612.5	610.5	430.3	426.6	434.7	433.4	433.1	431.9
619.6	619.3	609.1	608.7	625.2	624.7	623.6	612.7	610.7	438.2	436.5	439.9	437.7	446.1	444.1
619.7	619.3	609.2	608.7	625.4	624.9	623.7	612.9	610.8	446.5	441.5	461.1	460.2	460.2	459.4
645.8	645.5	631.1	630.0	656.5	655.2	652.3	643.4	638.0	458.4	454.1	466.4	464.5	469.4	467.8
727.1	725.6	718.5	717.7	712.8	710.0	705.5	717.4	710.0	461.8	460.5	470.6	469.1	469.7	468.6
727.2	725.6	718.7	717.7	712.9	710.1	705.7	717.7	710.4	471.8	468.9	479.9	479.0	481.0	480.1

727.3	725.6	718.9	717.7	713.0	710.2	705.8	717.8	710.5	472.5	470.0	485.5	484.3	487.0	486.0
727.4	725.6	720.7	721.6	713.1	710.3	705.9	718.5	718.4	476.2	474.9	487.6	485.6	495.9	494.5
749.6	754.2	720.8	721.6	740.3	736.2	743.5	718.6	718.4	496.0	493.8	494.3	492.9	503.8	502.0
749.8	754.2	720.9	721.6	740.3	736.2	743.6	718.8	718.6	503.0	498.7	510.3	508.5	510.7	508.9
750.0	754.2	722.7	725.4	740.6	736.5	743.8	727.5	731.0	510.1	507.5	523.6	521.8	524.0	524.2
750.0	754.2	722.8	725.4	754.2	751.4	762.3	727.7	731.1	512.7	509.0	523.9	523.4	528.6	527.1
750.1	754.2	723.1	725.4	754.2	751.5	762.5	728.0	731.4	521.2	517.1	535.2	532.8	533.5	532.0
762.6	764.8	723.1	725.4	754.6	751.8	762.7	728.0	731.4	542.5	537.8	547.6	544.5	551.4	549.0
762.7	764.8	723.2	725.4	754.6	751.9	762.7	728.1	731.5	550.4	551.2	563.7	563.2	563.2	562.1
762.8	764.8	745.5	743.9	754.7	752.0	762.9	741.3	734.4	576.3	573.7	572.7	570.2	572.2	569.9
782.6	782.4	745.7	743.9	777.0	774.7	769.3	741.5	734.6	576.3	573.7	577.2	575.8	574.3	574.1
782.9	782.4	745.8	743.9	777.3	775.0	769.6	741.6	734.7	586.1	584.6	580.2	580.2	576.1	574.9
782.9	782.4	745.9	743.9	777.4	775.0	769.7	741.7	734.7	587.6	586.2	596.8	594.6	596.6	594.4
811.3	810.6	751.9	751.0	816.5	812.9	805.2	760.4	751.3	602.4	600.7	603.1	601.7	600.1	601.1
811.6	810.6	752.0	751.0	816.8	813.2	805.4	760.6	751.5	612.7	610.6	606.7	607.0	602.6	601.2
811.7	810.6	752.4	751.0	817.0	813.4	805.6	760.9	751.7	613.0	611.8	608.0	608.1	605.1	604.9
812.2	810.6	753.0	751.0	817.4	813.8	806.0	761.5	752.4	614.3	614.6	611.9	609.3	607.7	605.2
830.2	832.8	786.4	788.1	844.7	845.5	847.6	796.4	797.8	626.1	627.6	620.0	619.6	618.7	617.4
830.3	832.8	786.4	788.1	844.7	845.6	847.7	796.4	797.9	634.2	631.4	637.3	635.0	636.5	634.2
830.5	832.8	786.7	788.1	844.9	845.8	847.9	796.7	798.1	647.6	645.6	647.4	645.6	645.5	644.3
830.6	832.8	786.8	788.1	845.1	845.9	848.0	796.8	798.2	652.2	648.9	652.3	649.7	650.6	648.1
923.3	924.5	862.1	861.1	923.4	923.9	925.8	878.1	869.6	655.6	649.1	659.6	658.4	652.3	653.2
923.5	924.5	862.5	861.1	923.7	924.2	926.0	878.5	870.1	672.9	671.4	661.4	660.9	662.5	660.1
923.7	924.5	862.7	861.1	923.9	924.4	926.3	878.7	870.3	681.5	673.4	688.7	686.6	681.8	681.5
923.8	924.5	862.8	861.1	924.0	924.5	926.4	878.8	870.4	684.4	676.3	706.9	704.3	699.2	699.1
925.9	925.8	863.0	861.1	948.4	945.8	940.1	878.9	870.5	718.3	716.0	713.6	714.6	708.8	710.1
926.4	925.8	884.1	883.7	948.9	946.3	940.6	899.7	893.7	719.1	718.6	717.0	716.4	710.7	713.7
926.5	925.8	884.2	883.7	949.0	946.5	940.7	899.8	893.8	724.4	725.1	719.0	719.3	719.2	716.8
926.6	925.8	884.4	883.7	949.1	946.6	940.9	900.0	894.1	749.7	746.0	738.0	737.4	736.6	734.6
926.7	925.8	884.6	883.7	949.2	946.7	940.9	900.1	894.2	754.6	754.5	752.1	750.6	748.4	747.4
945.3	945.5	884.7	883.7	957.6	960.0	960.2	900.3	894.3	779.4	779.3	783.3	782.8	774.9	773.8
945.4	945.5	917.1	917.3	957.7	960.2	960.4	920.3	919.9	792.9	790.9	786.5	785.2	780.6	779.4
945.6	945.5	917.2	917.3	957.9	960.3	960.6	920.4	919.9	798.2	798.4	788.2	787.9	790.2	790.1
945.7	945.5	917.4	917.3	966.7	964.5	960.7	920.6	920.2	801.1	800.3	795.5	795.0	790.8	790.3
945.8	945.5	917.6	917.3	966.8	964.7	960.8	920.8	920.3	821.6	818.4	813.2	811.9	806.7	805.5
958.9	962.2	942.6	944.7	967.0	964.9	966.7	944.9	951.6	823.5	822.0	818.0	816.4	809.0	807.3
959.0	962.2	942.8	944.7	967.1	965.0	966.8	945.1	951.8	827.1	826.0	821.7	819.2	816.0	814.3
959.1	962.2	943.0	944.7	967.3	965.1	967.0	945.3	951.9	835.3	832.8	826.3	824.5	821.2	818.8
1127.9	1134.3	1119.9	1126.4	1100.6	1106.6	1116.5	1095.4	1110.6	837.7	835.5	834.8	833.8	832.5	831.7
1127.9	1134.3	1120.0	1126.4	1100.7	1106.7	1116.5	1095.5	1110.6	861.6	859.6	849.5	848.2	839.0	838.1
1128.0	1134.3	1120.1	1126.4	1100.7	1106.7	1116.5	1095.6	1110.6	862.5	860.8	862.7	861.5	862.2	861.0
1128.0	1134.3	1120.1	1126.4	1100.8	1106.7	1116.7	1095.6	1110.9	870.0	868.6	864.7	864.0	862.7	862.1
1128.3	1134.3	1120.4	1126.4	1101.1	1107.0	1116.9	1095.9	1111.0	872.4	870.3	867.1	865.8	863.3	862.1
1129.2	1137.1	1122.1	1128.2	1106.4	1109.9	1120.9	1101.2	1113.9	888.0	886.4	884.6	883.9	864.4	863.4
1129.3	1137.1	1122.1	1128.2	1106.5	1110.0	1121.0	1101.4	1114.0	894.9	893.6	885.7	884.3	878.9	878.4
1129.4	1137.1	1122.3	1128.2	1106.7	1110.2	1121.1	1101.6	1114.1	897.6	896.1	901.8	900.9	896.8	896.7
1129.5	1137.1	1122.4	1128.2	1106.9	1110.3	1121.1	1101.7	1114.1	903.8	904.2	902.8	902.9	897.8	897.0
1129.8	1137.1	1122.7	1128.2	1107.1	1110.5	1121.2	1102.0	1114.3	908.2	908.1	904.2	904.2	902.1	902.1
1198.7	1213.5	1181.4	1195.1	1159.1	1167.3	1202.0	1149.0	1189.8	915.4	914.1	908.5	906.8	905.2	903.9
1198.8	1213.5	1181.6	1195.1	1159.2	1167.4	1202.1	1149.1	1189.8	925.4	921.6	912.7	911.4	911.6	910.0
1198.9	1213.5	1181.6	1195.1	1159.3	1167.5	1202.1	1149.2	1189.9	930.6	931.8	923.8	922.9	914.2	913.1
1216.0	1222.1	1198.9	1203.9	1192.8	1197.1	1209.7	1181.8	1196.4	933.6	933.3	940.6	941.1	935.7	934.5
1216.2	1222.1	1198.9	1203.9	1193.0	1197.2	1209.9	1181.9	1196.5	978.0	974.9	958.3	956.8	939.9	939.9
1216.3	1222.1	1199.1	1203.9	1193.1	1197.4	1210.0	1182.0	1196.7	983.9	982.3	960.1	957.9	947.2	945.7
1216.3	1222.1	1199.2	1203.9	1193.1	1197.4	1210.0	1182.1	1196.8	996.5	991.9	972.1	968.6	950.9	948.2
1262.2	1264.9	1246.4	1247.9	1250.4	1236.9	1256.9	1237.3	1242.0	997.2	995.5	986.6	984.3	973.0	971.1
1262.3	1264.9	1246.5	1247.9	1250.4	1236.9	1256.9	1237.3	1242.1	1014.7	1011.9	993.2	990.6	975.9	973.8
1262.4	1264.9	1246.6	1247.9	1250.6	1236.9	1257.0	1237.3	1242.1	1018.8	1015.6	995.8	992.9	984.3	982.6
1269.1	1270.8	1255.0	1255.9	1253.0	1252.0	1263.9	1238.0	1248.5	1022.6	1016.0	1001.3	999.4	985.6	982.9
1269.2	1270.8	1255.2	1255.9	1253.0	1252.1	1264.0	1238.1	1248.7	1041.5	1032.2	1007.4	1002.4	992.8	990.8
1269.3	1270.8	1255.3	1255.9	1253.0	1252.1	1264.0	1238.2	1248.7	1041.7	1035.1	1011.1	1008.5	993.2	991.8
1270.8	1272.7	1255.3	1256.3	1262.7	1263.5	1265.1	1248.7	1249.5	1045.2	1039.2	1024.9	1020.4	1000.9	998.7
1270.9	1272.7	1255.4	1256.3	1262.9	1263.7	1265.1	1248.8	1249.6	1051.0	1047.3	1038.2	1036.9	1035.5	1034.4
1271.0	1272.7	1255.5	1256.3	1263.0	1263.7	1265.2	1249.0	1249.6	1056.8	1049.5	1044.2	1042.7	1038.6	1037.3
1271.1	1272.7	1255.6	1256.3	1263.2	1264.1	1265.3	1249.0	1249.7	1059.7	1057.9	1052.9	1050.7	1045.2	1043.2
1271.1	1272.7	1255.6	1256.3	1263.3	1264.2	1265.3	1249.1	1249.8	1068.9	1066.2	1056.6	1053.3	1046.5	1043.6
1281.2	1284.3	1260.7	1263.0	1263.4	1264.3	1275.0	1249.2	1255.6	1083.0	1081.3	1076.8	1074.2	1067.0	1064.5
1281.2	1284.3	1260.8	1263.0	1263.4	1264.4	1275.0	1249.3	1255.7	1085.5	1084.5	1080.1	1075.7	1069.2	1065.7
1281.2	1284.3	1260.8	1263.0	1263.5	1264.4	1275.1	1249.3	1255.7	1088.8	1085.9	1081.2	1077.9	1074.3	1071.2
1281.3	1284.3	1260.9	1263.0	1268.8	1270.3	1275.1	1250.7	1255.7	1090.9	1086.6	1081.8	1080.7	1078.0	1075.6
1284.5	1291.0	1267.3	1272.5	1268.8	1270.3	1284.1	1250.7	1266.7	1095.7	1088.3	1083.1	1082.4	1079.9	1079.8
1284.6	1291.0	1267.3	1272.5	1268.8	1270.3	1284.1	1250.7	1266.7	1096.2	1096.4	1092.5	1092.6	1091.0	1090.1
1284.7	1291.0	1267.3	1272.5	1268.8	1270.3	1284.1	1250.7	1266.7	1108.4	1106.3	1097.7	1095.9	1091.2	1090.6
1295.9	1300.9	1276.3	1280.4	1279.5	1280.2	1293.3	1262.4	1273.5	1111.5	1106.9	1098.5	1098.0	1093.2	1090.8
1296.0	1300.9	1276.4	1280.4	1279.6	1280.3	1293.4	1262.5	1273.6	1117.8	1113.4	1101.4	1098.5	1094.6	1094.5
1296.1	1300.9	1276.5	1280.4	1279.7	1280.3	1293.4	1262.6	1273.7	1122.6	1119.0	1107.4	1105.7	1098.1	1096.2
1296.2	1300.9	1276.5	1280.4	1279.7	1280.4	1293.5	1262.6	1273.7	1124.2	1120.8	1108.8	1106.8	1103.1	1103.3
1296.2	1300.9	1276.6	1280.4	1279.8	1280.4	1293.5	1262.7	1273.7	1133.4	1129.0	1114.5	1112.2	1108.6	1107.2
3093.9	3129.4	3090.2	3123.1	2979.5	2996.8	3161.1	3025.0	3169.3	1143.9	1136.7	1136.5	1130.8	1129.3	1124.6
3094.0	3129.4	3090.2	3123.1	2979.5	2996.9	3161.1	3025.0	3169.4	1146.1	1138.7	1138.6	1132.6	1132.1	1126.6
3094.0	3129.4	3090.3	3123.1	2979.5	2997.0	3161.1	3025.0	3169.4	1155.2	1150.8	1146.9	1143.7	1137.3	1132.5
3096.1	3130.4	3092.4	3123.9	2979.5	2997.0	3162.0	3025.0	3170.1	1158.5	1154.8	1149.4	1146.4	1137.4	1134.4
3096.1	3130.4	3092.4	3123.9	2979.6	2997.1	3162.0	3025.1	3170.1	1167.2	1164.3	1154.7	1151.9	1140.5	1138.7
3096.1	3130.4	3092.4	3123.9	3021.8	3045.3	3162.0	3064.4	3170.1	1184.2	1175.6	1157.6	1152.6	1141.1	1138.8
3096.2	3130.4	3092.4	3123.9	3021.8	3045.3	3162.0	3064.4	3170.2	1184.3	1177.2	1169.2	1164.4	1158.4	1154.0
3096.5	3140.4	3092.5	3133.4	3021.9	3045.4	3168.5	3064.4	3176.7	1189.7	1186.9	1175.1	1169.7	1162.7	1158.4
3097.7	3140.4	3093.6	3133.4	3050.9	3086.0	3168.6	3075.8	3176.7	1193.5	1191.9	1189.5	1191.9	1189.7	1192.2
3097.7	3140.4	3093.7	3133.4	3051.0	3086.0	3168.6	3075.8	3176.8	1199.0	1196.5	1193.6	1195.9	1193.2	1196.0
3097.8	3140.4	3093.7	3133.4	3051.0	3086.1	3168.6	3075.9	3176.8	1216.9	1219.5	1215.4	1218.3	1214.2	1217.2
3097.8	3146.8	3093.8	3139.1	3051.1	3086.3	3173.1	3075.9	3180.9	1221.5	1220.1	1220.4	1220.0	1219.3	1220.1
3103.1	3146.8	3099.0	3139.1	3052.4	3086.4	3173.2	3075.9	3180.9	1222.1	1222.0	1221.8	1222.0	1221.7	1221.0
3103.2	3146.8	3099.1	3139.1	3052.4	3086.4	3173.2	3076.0	3180.9	1222.2	1223.2	1222.2	1222.3	1222.4	1222.6
3103.2	3146.8	3099.1	3139.1	3052.5	3086.4	3173.2	3076.0	3181.0	1232.5	1231.4	1230.4	1230.2	1229.0	1229.1
3103.3	3146.8	3099.2	3139.1	3055.2	3091.4	3173.3	3079.7	3181.0	1233.4	1234.0	1231.9	1233.3	1230.0	1231.5
3108.8	3156.2	3110.1	3147.6	3059.9	3091.5	3180.3	3083.3	3187.9	1238.4	1239.3	1237.8	1238.7	1236.5	1237.4
3108.9	3156.2	3110.1	3147.6	3060.0	3091.5	3180.3	3083.3	3187.9	1246.1	1246.8	1245.1	1245.6	1242.8	1243.3
3109.1	3156.2	3110.1	3147.6	3060.0	3091.5	3180.3	3083.3	3188.0	1269.5	1270.0	1264.4	1266.0	1258.2	1260.2
3116.1	3163.4	3113.4	3156.0	3060.1	3102.1	3184.4	3083.4	3191.6	1271.0	1271.7	1264.8	1266.6	1260.1	1262.2
									1274.6	1278.7	1271.5	1276.1	1267.8	1272.9
									1280.9	1282.2	1275.8	1277.9	1270.5	1272.9
									1285.9	1289.6	1283.5	1286.4	1278.9	1280.4
									1287.8	1290.6	1286.1	1288.6	1280.8	1283.1
									1294.9	1296.0	1287.5	1289.1	1283.5	1286.7
									1295.0	1297.0	1290.6	1293.2	1284.5	1288.3
									1295.1	1297.0	1291.2	1294.6	1287.1	1289.5
									1297.0	1298.3	1294.0	1295.4	1289.6	1292.7

									1301.9	1303.6	1298.7	1300.7	1291.9	1294.4
									1305.9	1306.5	1299.4	1301.7	1292.9	1295.4
									1306.1	1307.7	1299.5	1302.4	1293.1	1295.7
									1306.4	1309.6	1301.3	1305.2	1296.5	1300.8
									1310.1	1312.6	1302.0	1305.9	1298.6	1302.1
									1311.0	1313.2	1306.1	1309.5	1302.9	1306.8
									1313.4	1315.7	1308.4	1310.1	1305.1	1307.5
									1314.2	1315.8	1309.4	1310.3	1306.0	1308.1
									1315.2	1316.4	1312.6	1314.7	1311.3	1313.3
									1317.6	1318.7	1312.9	1315.2	1312.1	1313.6
									1318.6	1322.0	1313.9	1315.6	1312.7	1314.1
									1319.8	1322.6	1318.0	1320.9	1314.9	1318.0
									1321.3	1323.6	1318.8	1321.8	1318.3	1320.9
									1323.0	1329.2	1319.4	1323.0	1318.6	1321.2
									1328.1	1331.3	1325.3	1326.2	1320.0	1321.4
									1330.3	1332.3	1325.8	1327.7	1323.7	1325.7
									1331.1	1334.9	1327.9	1331.8	1324.0	1328.0
									1332.8	1337.5	1330.3	1333.6	1328.1	1330.2
									1337.5	1338.4	1332.1	1333.8	1328.7	1331.4
									1337.5	1339.0	1334.0	1336.3	1331.1	1333.6
									1337.7	1340.5	1334.6	1337.4	1331.4	1333.8
									1345.0	1345.2	1340.6	1342.6	1337.6	1340.2
									1345.1	1346.6	1341.4	1342.9	1338.7	1340.5
									1345.5	1346.7	1342.5	1343.8	1340.2	1341.4
									1355.0	1357.9	1352.5	1355.4	1346.8	1349.9
									1359.4	1361.5	1355.3	1356.3	1349.8	1350.8
									1361.1	1362.0	1357.3	1359.2	1353.7	1354.8
									1362.3	1363.5	1358.0	1359.8	1354.7	1356.4
									1363.2	1365.5	1360.1	1361.8	1355.8	1357.8
									1366.2	1367.8	1363.3	1364.4	1356.3	1359.1
									1366.6	1368.9	1364.0	1366.1	1356.6	1359.3
									1367.9	1372.1	1364.3	1366.3	1358.4	1360.2
									1371.0	1373.1	1365.9	1366.6	1359.1	1360.7
									1372.8	1373.4	1365.9	1368.0	1360.0	1361.3
									1373.1	1373.8	1367.2	1368.3	1360.6	1361.3
									1373.7	1375.5	1368.1	1369.3	1361.1	1362.3
									1375.6	1376.0	1369.8	1371.5	1363.2	1364.3
									1377.0	1378.7	1372.0	1372.8	1366.7	1368.8
									1379.9	1382.4	1372.5	1374.1	1367.1	1369.8
									1382.5	1383.0	1376.6	1378.7	1367.4	1370.2
									1385.0	1386.2	1378.7	1380.2	1369.7	1373.0
									1385.3	1388.6	1380.5	1383.0	1371.4	1374.4
									1391.9	1393.8	1384.6	1388.2	1374.0	1375.4
									1399.7	1401.2	1387.3	1388.7	1375.3	1377.0
									1401.1	1401.4	1387.4	1388.9	1375.5	1377.6
									1402.3	1407.9	1389.1	1391.2	1378.9	1380.3
									1407.1	1409.5	1389.7	1392.7	1381.1	1383.6
									1411.4	1413.2	1394.6	1397.9	1385.4	1387.0
									1415.5	1417.2	1396.0	1398.4	1387.8	1389.3
									1416.9	1418.2	1400.7	1402.5	1389.6	1391.3
									1441.1	1448.7	1400.9	1403.2	1392.1	1392.5
									1442.0	1449.5	1402.3	1403.7	1394.4	1397.0
									2968.8	3032.9	2993.7	3041.3	3000.4	3044.4
									2971.2	3033.3	2995.3	3041.8	3002.5	3045.0
									2980.0	3046.5	3001.1	3052.0	3004.1	3053.2
									2982.0	3047.4	3002.9	3052.3	3006.7	3054.2
									2985.0	3048.1	3004.5	3054.4	3006.8	3055.3
									2990.1	3051.1	3006.4	3055.2	3009.7	3056.9
									2991.8	3052.5	3007.4	3056.2	3010.8	3057.3
									2992.4	3054.3	3009.3	3057.5	3011.4	3058.1
									2993.9	3056.4	3009.6	3060.0	3012.8	3061.4
									2995.8	3056.6	3012.1	3062.9	3016.7	3065.2
									2996.8	3062.4	3014.3	3065.2	3018.7	3065.5
									2999.6	3063.7	3016.4	3066.2	3020.4	3066.2
									3007.4	3065.0	3020.4	3068.3	3021.7	3069.3
									3009.4	3067.5	3021.3	3071.0	3023.4	3071.9
									3009.6	3071.2	3023.3	3077.4	3025.5	3078.0
									3011.7	3075.8	3024.3	3080.7	3025.6	3081.0
									3012.1	3077.6	3025.7	3081.2	3031.1	3081.4
									3013.2	3078.5	3026.8	3081.4	3031.4	3081.7
									3016.3	3078.6	3029.2	3082.3	3032.3	3082.7
									3016.5	3079.5	3029.2	3083.0	3036.8	3082.8
									3018.6	3080.9	3030.4	3083.1	3037.6	3084.2
									3019.8	3081.9	3032.0	3085.4	3038.0	3086.1
									3024.7	3083.4	3033.3	3087.3	3038.4	3087.4
									3027.5	3087.5	3038.0	3092.6	3038.9	3093.3
									3028.5	3090.8	3039.2	3094.6	3039.7	3093.8
									3028.6	3090.9	3040.0	3094.7	3039.9	3095.3
									3028.7	3093.1	3040.5	3096.9	3040.8	3098.2
									3042.3	3095.9	3044.6	3098.4	3045.2	3098.6
									3043.5	3097.4	3047.8	3101.2	3045.4	3102.1
									3043.9	3098.6	3048.0	3102.7	3046.7	3103.8
									3044.6	3106.8	3053.7	3109.6	3050.9	3109.2
									3049.8	3108.4	3059.0	3109.8	3057.5	3109.4
									3053.3	3110.5	3059.2	3113.3	3065.3	3112.6
									3053.3	3110.9	3062.0	3115.0	3069.2	3114.1
									3060.8	3137.8	3084.0	3135.3	3090.9	3129.7
									3069.0	3138.9	3086.8	3136.6	3091.1	3131.7

Table S4. Vertical electron attachment energies (eV) and pole strengths (in parentheses) of $K@C_{20}H_{20}^{+}$, at neutral $K@C_{20}H_{20}$ geometry (optimized at B3LYP/aug-cc-pVTZ level) obtained from diagonal electron propagator methods using cc-pVTZ (K, C) and d-aug-cc-pVTZ (H). All valence electrons are correlated.

Final State	Vertical electron attachment energies and pole strengths			
(I_h)	KT	D2 (PS)	P3 (PS)	P3+ (PS)
1^2A_g	-1.765	-2.153 (0.985)	-2.115 (0.986)	-2.120 (0.985)
1^2T_{1u}	-1.547	-1.855 (0.988)	-1.831 (0.988)	-1.834 (0.988)
1^2H_g	-1.200	-1.412 (0.992)	-1.399 (0.991)	-1.400 (0.991)
1^2T_{2u}	-0.807	-0.953 (0.994)	-0.943 (0.994)	-0.944 (0.994)
1^2G_u	-0.782	-0.880 (0.996)	-0.877 (0.996)	-0.878 (0.996)
2^2A_g	-0.738	-0.994 (0.990)	-0.961 (0.991)	-0.965 (0.991)
2^2T_{1u}	-0.664	-0.889 (0.991)	-0.864 (0.992)	-0.867 (0.992)
1^2G_g	-0.398	-0.441 (0.998)	-0.441 (0.998)	-0.441 (0.998)
2^2H_g	-0.364	-0.610 (0.990)	-0.587 (0.991)	-0.590 (0.991)
2^2T_{2u}	0.062	-0.338 (0.985)	-0.291 (0.986)	-0.296 (0.986)
2^2G_u	0.097	-0.126 (0.991)	-0.115 (0.991)	-0.116 (0.991)

Table S5. Vertical electron attachment energies (eV) and pole strengths (in parentheses) of $Rb@C_{20}H_{20}^{+}$ at neutral $Rb@C_{20}H_{20}$ geometry, obtained from diagonal electron propagator methods using cc-pVTZ (C), d-aug-cc-pVTZ (H), and cc-pVTZ-PP (Rb) (Rb: 28 ECP). All valence electrons are correlated.

Final state	Vertical electron attachment energies and pole strengths			
(I_h)	KT	D2 (PS)	P3 (PS)	P3+ (PS)
1^2A_g	-1.738	-2.100 (0.986)	-2.060 (0.987)	-2.065 (0.987)
1^2T_{1u}	-1.530	-1.827 (0.988)	-1.796 (0.989)	-1.800 (0.988)
1^2H_g	-1.198	-1.408 (0.992)	-1.390 (0.992)	-1.392 (0.992)
1^2T_{2u}	-0.808	-0.956 (0.994)	-0.942 (0.994)	-0.944 (0.994)
1^2G_u	-0.781	-0.881 (0.996)	-0.876 (0.996)	-0.876 (0.996)
2^2A_g	-0.735	-0.969 (0.991)	-0.936 (0.992)	-0.940 (0.992)
2^2T_{1u}	-0.651	-0.880 (0.991)	-0.849 (0.992)	-0.853 (0.992)
1^2G_g	-0.399	-0.444 (0.998)	-0.442 (0.998)	-0.442 (0.998)
2^2H_g	-0.377	-0.612 (0.991)	-0.585 (0.991)	-0.588 (0.991)
2^2T_{2u}	0.056	-0.347 (0.985)	-0.289 (0.986)	-0.297 (0.986)
2^2G_u	0.092	-0.129 (0.991)	-0.113 (0.991)	-0.114 (0.991)

Table S6. Vertical electron attachment energies (eV) and pole strengths (in parentheses) of $Ca@C_{20}H_{20}^{2+}$ at neutral $Ca@C_{20}H_{20}^{+}$ geometry, obtained from diagonal electron propagator methods using cc-pVTZ (Ca, C) and d-aug-cc-pVTZ (H). All valence electrons are correlated.

Final state (I_h)	Vertical electron attachment energies and pole strengths			
	KT	D2 (PS)	P3 (PS)	P3+ (PS)
1^2A_g	-4.417	-5.210 (0.972)	-5.098 (0.974)	-5.113 (0.974)
1^2T_{1u}	-4.068	-4.743 (0.975)	-4.663 (0.977)	-4.672 (0.976)
1^2H_g	-3.563	-4.153 (0.979)	-4.078 (0.980)	-4.088 (0.980)
1^2T_{2u}	-3.082	-3.765 (0.976)	-3.670 (0.978)	-3.683 (0.978)

Table S7. Vertical electron attachment energies (eV) and pole strengths (in parentheses) of $Na@C_{36}H_{36}^{+}$ at neutral $Na@C_{36}H_{36}$ geometry, obtained from diagonal electron propagator methods using cc-pVDZ (Na, C) and d-aug-cc-pVDZ (H). All valence electrons are correlated.

Final state (D_2)	Vertical electron attachment energies and pole strengths			
	KT	D2 (PS)	P3 (PS)	P3+ (PS)
1^2A	-1.723	-2.490 (0.972)	-2.356 (0.975)	-2.375 (0.975)
1^2B_1	-1.463	-1.887 (0.984)	-1.855 (0.983)	-1.859 (0.983)
1^2B_2	-1.444	-1.882 (0.983)	-1.846 (0.983)	-1.850 (0.983)
1^2B_3	-1.365	-1.800 (0.983)	-1.757 (0.984)	-1.762 (0.984)
2^2B_3	-1.118	-1.392 (0.989)	-1.380 (0.988)	-1.382 (0.988)
2^2A	-1.115	-1.385 (0.989)	-1.373 (0.989)	-1.375 (0.989)
2^2B_2	-1.081	-1.341 (0.990)	-1.333 (0.989)	-1.334 (0.989)
2^2B_1	-1.075	-1.343 (0.989)	-1.334 (0.989)	-1.335 (0.989)
3^2A	-1.072	-1.350 (0.989)	-1.340 (0.988)	-1.341 (0.988)

Table S8. Vertical electron attachment energies (eV) and pole strengths (in parentheses) of $K@C_{36}H_{36}^{+}$ at neutral $K@C_{36}H_{36}$ geometry, obtained from diagonal electron propagator methods using cc-pVDZ (K, C) and d-aug-cc-pVDZ (H). All valence electrons are correlated.

Final state (D_2)	Vertical electron attachment energies and pole strengths			
	KT	D2 (PS)	P3 (PS)	P3+ (PS)
1^2A	-1.636	-2.228 (0.978)	-2.150 (0.979)	-2.161 (0.979)
1^2B_1	-1.430	-1.812 (0.985)	-1.785 (0.985)	-1.788 (0.985)
1^2B_2	-1.425	-1.823 (0.985)	-1.794 (0.984)	-1.797 (0.984)
1^2B_3	-1.350	-1.750 (0.985)	-1.717 (0.984)	-1.721 (0.984)
2^2B_3	-1.122	-1.394 (0.989)	-1.379 (0.989)	-1.381 (0.989)
2^2A	-1.118	-1.388 (0.989)	-1.374 (0.989)	-1.375 (0.989)
2^2B_1	-1.084	-1.352 (0.990)	-1.340 (0.989)	-1.342 (0.989)
2^2B_2	-1.084	-1.346 (0.990)	-1.335 (0.989)	-1.336 (0.989)
3^2A	-1.073	-1.340 (0.990)	-1.330 (0.989)	-1.331 (0.989)

Table S9. Vertical electron attachment energies (eV) and pole strengths (in parentheses) of $Rb@C_{36}H_{36}^{+}$ at neutral $Rb@C_{36}H_{36}$ geometry, obtained from diagonal electron propagator methods using cc-pVDZ (C), d-aug-cc-pVDZ (H), and cc-pVDZ-PP (Rb) (Rb: 28 ECP). All valence electrons are correlated.

Final state (D_2)	Vertical electron attachment energies and pole strengths			
	KT	D2 (PS)	P3 (PS)	P3+ (PS)
1^2A	-1.617	-2.167 (0.979)	-2.098 (0.980)	-2.107 (0.980)
1^2B_1	-1.414	-1.777 (0.986)	-1.751 (0.985)	-1.754 (0.985)
1^2B_2	-1.413	-1.795 (0.985)	-1.766 (0.985)	-1.770 (0.985)
1^2B_3	-1.345	-1.720 (0.986)	-1.692 (0.985)	-1.695 (0.985)
2^2B_3	-1.116	-1.404 (0.989)	-1.385 (0.988)	-1.388 (0.988)
2^2A	-1.113	-1.399 (0.989)	-1.381 (0.988)	-1.383 (0.988)
2^2B_1	-1.083	-1.365 (0.989)	-1.350 (0.988)	-1.352 (0.988)
2^2B_2	-1.082	-1.355 (0.989)	-1.341 (0.989)	-1.343 (0.989)
3^2A	-1.072	-1.347 (0.989)	-1.334 (0.988)	-1.335 (0.989)